```
=> log y
COST IN U.S. DOLLARS                              SINCE FILE     TOTAL
                                                       ENTRY   SESSION
FULL ESTIMATED COST                                   293.70    460.85

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE     TOTAL
                                                       ENTRY   SESSION
CA SUBSCRIBER PRICE                                   -41.25    -41.25

STN INTERNATIONAL LOGOFF AT 11:03:09 ON 04 MAY 2006
```

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LOGINID:SSPTANAG1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1          Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2          "Ask CAS" for self-help around the clock
 NEWS  3  DEC 23  New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/
                  USPAT2
 NEWS  4  JAN 13  IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
 NEWS  5  JAN 13  New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to
                  INPADOC
 NEWS  6  JAN 17  Pre-1988 INPI data added to MARPAT
 NEWS  7  JAN 17  IPC 8 in the WPI family of databases including WPIFV
 NEWS  8  JAN 30  Saved answer limit increased
 NEWS  9  FEB 21  STN AnaVist, Version 1.1, lets you share your STN AnaVist
                  visualization results
 NEWS 10  FEB 22  The IPC thesaurus added to additional patent databases on STN
 NEWS 11  FEB 22  Updates in EPFULL; IPC 8 enhancements added
 NEWS 12  FEB 27  New STN AnaVist pricing effective March 1, 2006
 NEWS 13  FEB 28  MEDLINE/LMEDLINE reload improves functionality
 NEWS 14  FEB 28  TOXCENTER reloaded with enhancements
 NEWS 15  FEB 28  REGISTRY/ZREGISTRY enhanced with more experimental spectral
                  property data
 NEWS 16  MAR 01  INSPEC reloaded and enhanced
 NEWS 17  MAR 03  Updates in PATDPA; addition of IPC 8 data without attributes
 NEWS 18  MAR 08  X.25 communication option no longer available after June 2006
 NEWS 19  MAR 22  EMBASE is now updated on a daily basis
 NEWS 20  APR 03  New IPC 8 fields and IPC thesaurus added to PATDPAFULL
 NEWS 21  APR 03  Bibliographic data updates resume; new IPC 8 fields and IPC
                  thesaurus added in PCTFULL
 NEWS 22  APR 04  STN AnaVist $500 visualization usage credit offered
 NEWS 23  APR 12  LINSPEC, learning database for INSPEC, reloaded and enhanced
 NEWS 24  APR 12  Improved structure highlighting in FQHIT and QHIT display
                  in MARPAT
 NEWS 25  APR 12  Derwent World Patents Index to be reloaded and enhanced during
                  second quarter; strategies may be affected

 NEWS EXPRESS  FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
               V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT
               http://download.cas.org/express/v8.0-Discover/

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
specific topic.
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FILE 'HOME' ENTERED AT 10:59:26 ON 04 MAY 2006

=> fil reg
COST IN U.S. DOLLARS                                 SINCE FILE       TOTAL
                                                          ENTRY     SESSION
FULL ESTIMATED COST                                        0.21        0.21

FILE 'REGISTRY' ENTERED AT 10:59:33 ON 04 MAY 2006
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STRUCTURE FILE UPDATES:     3 MAY 2006  HIGHEST RN 882736-15-4
DICTIONARY FILE UPDATES:    3 MAY 2006  HIGHEST RN 882736-15-4

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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*******************************************************************
*                                                                 *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                 *
*******************************************************************
```

```
Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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Uploading C:\Program Files\Stnexp\Queries\10955129amend.str
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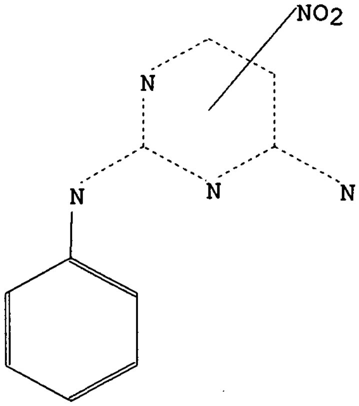

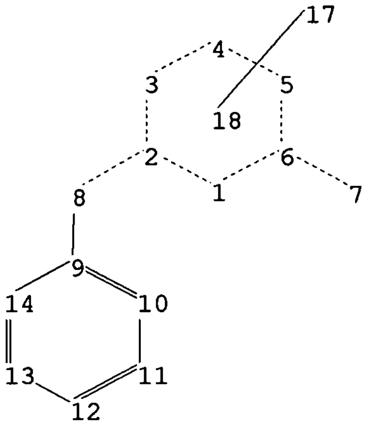

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chain nodes :
7  8  17
ring nodes :
1  2  3  4  5  6  9  10  11  12  13  14
chain bonds :
2-8  6-7  8-9
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  9-10  9-14  10-11  11-12  12-13  13-14
exact/norm bonds :
1-2  1-6  2-3  2-8  3-4  4-5  5-6  6-7  8-9
normalized bonds :
9-10  9-14  10-11  11-12  12-13  13-14
isolated ring systems :
containing 1 :


G1:C,O,S,N

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  17:CLASS  18:CLASS




L1      STRUCTURE UPLOADED

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L1 HAS NO ANSWERS
L1              STR
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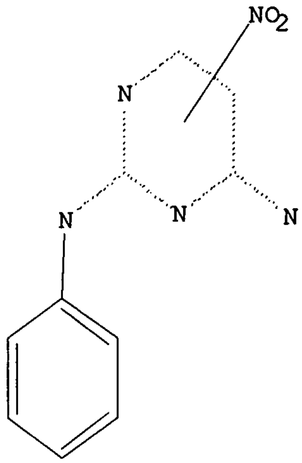

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G1 C,O,S,N


Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 11:00:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      156 TO ITERATE

100.0% PROCESSED      156 ITERATIONS                            50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:         2371 TO     3869
PROJECTED ANSWERS:             608 TO     1472

L2           50 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 11:00:09 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     3308 TO ITERATE

100.0% PROCESSED     3308 ITERATIONS                          1159 ANSWERS
SEARCH TIME: 00.00.01

L3         1159 SEA SSS FUL L1

=> fil hcaplus
COST IN U.S. DOLLARS                              SINCE FILE     TOTAL
                                                       ENTRY   SESSION
FULL ESTIMATED COST                                   166.94    167.15

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FILE LAST UPDATED: 3 May 2006  (20060503/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> s l3
L4          57 L3

=> s l4 and (fluorescent or label or fluoresc?)
        151385 FLUORESCENT
         60348 LABEL
        441092 FLUORESC?
L5           1 L4 AND (FLUORESCENT OR LABEL OR FLUORESC?)

=> d ed abs ibib hitstr
```

L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 15 Apr 2005
AB The invention provides methods relating to a novel screening assay format that can be applied to broad members of the protein kinase gene family. More specifically, the assay was used for inhibitors of STK12 kinase domain. The assay uses a series of **fluorescently** labeled, active site probes described herein that can be displaced by an inhibitor agent. The Kd for the inhibitor compound is derived based on the Kd of the probe for the kinase and the dose response of the inhibitor agent. The invention also provides novel active site probes suitable for use with the screening method.

```
ACCESSION NUMBER:        2005:324323  HCAPLUS
DOCUMENT NUMBER:         142:367631
TITLE:                   Fluorescent probes for use in protein kinase
                         inhibitor binding competition assay for screening
                         applications
INVENTOR(S):             Prokopowicz, Anthony S.; Brown, Martha Priscilla;
                         Wildeson, Jessi Marie; Jakes, Scott; Labadia, Mark E.
PATENT ASSIGNEE(S):      Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE:                  PCT Int. Appl., 49 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                English
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE       APPLICATION NO.        DATE
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     WO 2005033330        A2    20050414   WO 2004-US32253        20040930
     WO 2005033330        A3    20050728
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
     US 2005100978        A1    20050512   US 2004-955129         20040930
PRIORITY APPLN. INFO.:                     US 2003-508539P     P  20031003
OTHER SOURCE(S):         MARPAT 142:367631
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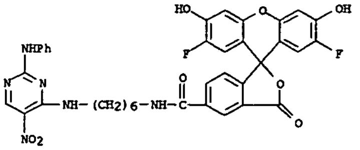
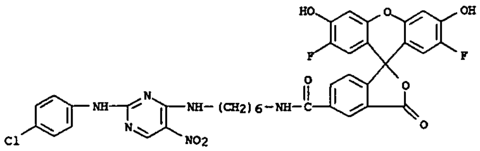
IT **849339-53-3 849339-54-4 849339-55-5**
849339-56-6 849339-57-7
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(**fluorescent** probe; **fluorescent** probes for use in protein kinase inhibitor binding competition assay for screening applications)
RN 849339-53-3 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxamide, 2',7'-difluoro-3',6'-dihydroxy-N-[6-[[5-nitro-2-(phenylamino)-4-pyrimidinyl]amino]hexyl]-3-oxo- (9CI) (CA INDEX NAME)

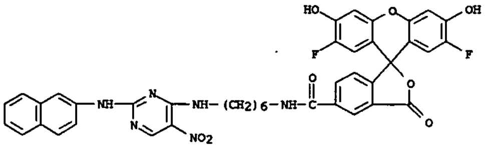
L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 849339-54-4 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxamide, N-[6-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]hexyl]-2',7'-difluoro-3',6'-dihydroxy-3-oxo- (9CI) (CA INDEX NAME)

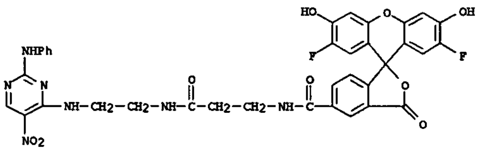


RN 849339-55-5 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxamide, 2',7'-difluoro-3',6'-dihydroxy-N-[6-[[2-(2-naphthalenylamino)-5-nitro-4-pyrimidinyl]amino]hexyl]-3-oxo- (9CI) (CA INDEX NAME)



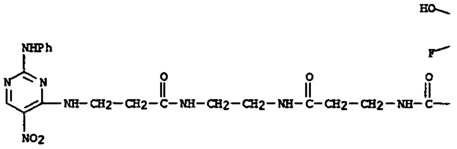
RN 849339-56-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxamide, 2',7'-difluoro-3',6'-dihydroxy-N-[3-[[2-[[5-nitro-2-(phenylamino)-4-pyrimidinyl]amino]ethyl]amino]-3-oxopropyl]-3-oxo- (9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

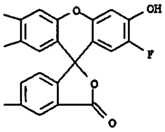


RN 849339-57-7 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxamide, 2',7'-difluoro-3',6'-dihydroxy-N-[3-[[2-[[3-[[5-nitro-2-(phenylamino)-4-pyrimidinyl]amino]-1-oxopropyl]amino]ethyl]amino]-3-oxopropyl]-3-oxo- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



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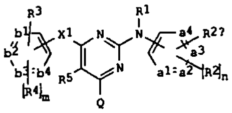
L4 ANSWER 1 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 06 Apr 2006
GI



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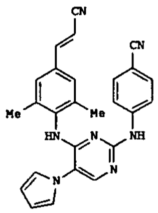

II

AB HIV replication inhibitors I [-a1=a2-a3=a4- = -CH=CH-CH=CH-, -N=CH-CH=CH-, -N=CH-N=CH-, -N=CH-CH=N-, -N=N-CH=CH-; -b1=b2-b3=b4- = -CH=CH-CH=CH-, -N=CH-CH=CH-, -N=CH-N=CH-, -N=CH-CH=N-, -N=N-CH=CH-; R1 = H, aryl, formyl, alkylcarbonyl, etc.; R2 = OH, halo, (un)substituted alkyl, alkenyl, etc.; R2a = CN, (un)substituted amino, (un)substituted alkyl, etc.; X1 = NR1, O, C(O), CH2, CHOH, S, S(O)p; R3 = CN, amino, alkyl, etc.; R4 = halo, OH, (un)substituted alkyl, alkenyl, etc.; R5 = 5-6 membered completely unsatd. ring system wherein 1-4 ring members are N, O or S, which ring may optionally be substituted and may optionally be annelated with a benzene ring; Q = H, alkyl, halo, etc.; n, m = 0-4; p = 1-2; and N-oxides, pharmaceutically acceptable addition salts, quaternary amines or stereoisomeric forms thereof]. E.g., a multi-step synthesis of II, starting from 2,4-dichloro-5-nitropyrimidine and 4-(2-cyanoethenyl)-2,6-dimethylphenylamine, was given. The antiviral activity of the compds. I was evaluated in the presence of the wild type HIV and HIV mutants bearing mutations at the reverse transcriptase gene (data given). The invention also relates to the use of compds. I for the prevention or the treatment of HIV infection.

ACCESSION NUMBER:	2006:318550 HCAPLUS
TITLE:	Preparation of HIV inhibiting 5-heterocyclyl pyrimidines
INVENTOR(S):	Guillemont, Jerome Emile Georges; Heeres, Jan; Lewi, Paulus Joannes
PATENT ASSIGNEE(S):	Tibotec Pharmaceuticals Ltd., Ire.

L4 ANSWER 1 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

SOURCE:	PCT Int. Appl., 67 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

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     PATENT NO.          KIND    DATE        APPLICATION NO.         DATE
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     WO 2006035067        A2     20060406    WO 2005-EP54930         20050929
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
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             LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ,
             NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG,
             SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN,
             YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.:                       EP 2004-104812      A  20040930
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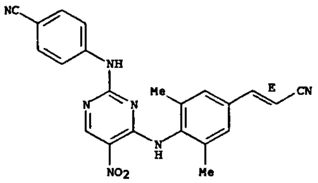
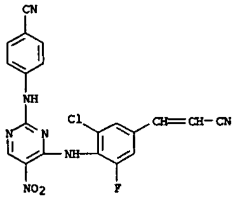
IT **882054-54-8P 882054-57-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of HIV inhibiting 5-heterocyclyl pyrimidines)
RN 882054-54-8 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.

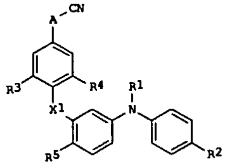


RN 882054-57-1 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED

L4 ANSWER 1 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



L4 ANSWER 2 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 06 Apr 2006
GI



I

AB 5-substituted pyrimidines HIV replication inhibitors [I; A = CH2CH2, CH:CH, C.tplbond.C; R1 = hydrogen, aryl, formyl, C1-6 alkylcarbonyl, C1-6 alkyl, C1-6 (alkyloxy)carbonyl; R2 = hydroxy, halo, C1-6 alkyl, carboxyl, cyano, C(:O)R6, nitro, (un)substituted amino, polyhalomethyl; X1 = NR1, O, S, S(:O)p; R3, R4 = H, C1-6 alkyl, halogen; R5 = nitro, (un)substituted amino, aryl, halogen, CHO, COR6, CO2R7, NHCHO, -NHC(:O)R6, CH:NOR8; R6 = C1-4 alkyl, (un)substituted amino, polyhalo C1-4 alkyl; R7 = hydrogen, C1-6 alkyl, arylalkyl; R8 = hydrogen, C1-6 alkyl, aryl; p = 1,2], which demonstrate HIV reverse transcriptase inhibition, are prepared and pharmaceutical compns. containing them are presented.

ACCESSION NUMBER:	2006:318326 HCAPLUS
TITLE:	Preparation of HIV-inhibiting 5-substituted pyrimidines
INVENTOR(S):	Guillemont, Jerome Emile Georges; Heeres, Jan; Lewi, Paulus Joannes
PATENT ASSIGNEE(S):	Tibotec Pharmaceuticals Ltd., Ire.
SOURCE:	PCT Int. Appl., 49 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

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     WO 2006035069        A1     20060406    WO 2005-EP54932         20050929
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ,
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             YU, ZA, ZM, ZW
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             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.:                       EP 2004-104805      A  20040930
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IT **882054-54-8P 882187-00-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

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L4   ANSWER 2 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
     (Reactant or reagent)
        (in the prepn. of HIV-inhibiting 5-substituted pyrimidines)
RN   882054-54-8  HCAPLUS
CN   INDEX NAME NOT YET ASSIGNED
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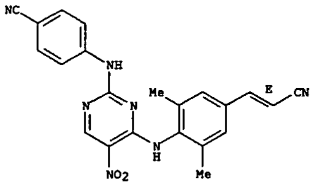
Double bond geometry as shown.



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RN   882187-00-0  HCAPLUS
CN   INDEX NAME NOT YET ASSIGNED
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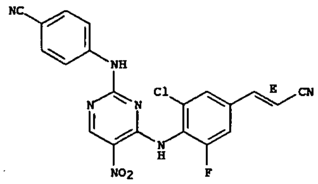
Double bond geometry as shown.



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REFERENCE COUNT:        2        THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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L4   ANSWER 3 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  06 Apr 2006
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

AB   The title compds. I [-a1=a2-a3=a4- = -CH=CH-CH=CH-, -N=CH-CH=CH-,
     -N=CH-N=CH-, -N=CH-CH=N-, -N=N-CH=CH-; -b1=b2-b3=b4- = -CH=CH-CH=CH-,
     -N=CH-CH=CH-, -N=CH-N=CH-, -N=CH-CH=N-, -N=N-CH=CH-; R1' = H, aryl, formyl,
     alkylcarbonyl, (un)substituted alkyl, alkyloxycarbonyl; R2 = OH, halo,
     (un)substituted alkyl, alkenyl or alkynyl, etc.; R2a = CN, (un)substituted
     amino, (un)substituted alkyl, halo, etc.; X1 = NR1, O, C(O), CH2, CHOH, S,
     S(O)r; R3 = CN, amino, alkyl, halo, etc.; R4 = halo, OH, (un)substituted
     alkyl, alkenyl or alkynyl, etc.; R5 = Y(Alk)L, (Alk')YL, (Alk')Y(Alk)L
     (wherein Alk or Alk' = bivalent alkyl or alkenyl; L = aryl, Het; Y = O, S,
     S(O)r, NR1, CH=N-O; Het = 5-6 membered completely unsatd. ring wherein 1-4
     ring members are heteroatoms); Q = H, alkyl, halo, etc.; m, n = 0-4; and
     their N-oxides, a pharmaceutically acceptable addition salts, a quaternary
     amines or a stereoisomeric forms], useful as HIV replication inhibitors,
     were prepared and formulated.  E.g., a multi-step synthesis of II, starting
     from 2,4-dichloro-5-nitropyrimidine and 4-(2-cyanoethenyl)-2,6-
     dimethylphenylamine, was given.  The compds. I were tested for their
     potency against clin. isolated HIV strains harboring several mutations
     (data given for representative compds. I).  Processes for the preparation of
     compds. I, pharmaceutical compns. comprising I as active ingredient and
     the use of compds. I for the prevention or the treatment of HIV infection
     were disclosed.
ACCESSION NUMBER:        2006:317260  HCAPLUS
TITLE:                   Preparation of HIV inhibiting 5-carbo- or heterocyclic
                         substituted pyrimidines
INVENTOR(S):             Guillemont, Jerome Emile Georges; Heeres, Jan; Lewi,
                         Paulus Joannes
PATENT ASSIGNEE(S):      Tibotec Pharmaceuticals Ltd., Ire.
SOURCE:                  PCT Int. Appl., 74 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                English
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND    DATE        APPLICATION NO.         DATE
     ---------------     ----    --------    --------------------    --------
     WO 2006035068        A2     20060406    WO 2005-EP54931         20050929
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ,
             NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG,
             SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN,
             YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.:                       EP 2004-104814      A  20040930
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L4   ANSWER 3 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
IT   882054-54-8P 882187-00-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of HIV inhibiting 5-carbo- or heterocyclic substituted
        pyrimidines)
RN   882054-54-8  HCAPLUS
CN   INDEX NAME NOT YET ASSIGNED
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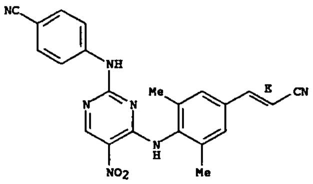
Double bond geometry as shown.



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RN   882187-00-0  HCAPLUS
CN   INDEX NAME NOT YET ASSIGNED
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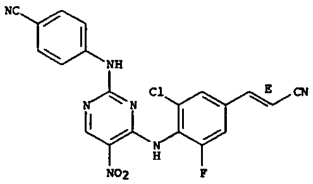
Double bond geometry as shown.



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L4   ANSWER 4 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  03 Mar 2006
GI
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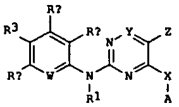

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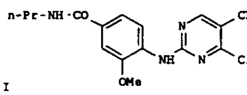

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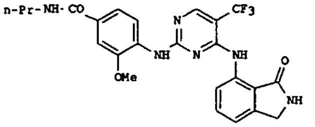

III

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AB   Title compds. I [W = N, CR2; X = O, S, NR1a; Y = CH, N; Z = H, halo, NO2,
     etc.; A = mono or bicyclic aryl ring (sic); R1, R1a = H, CH3; R2 = H,
     halo, OR4, etc.; Ra, Rb, Rc = H, halo, =O, etc.; R4 = H, alkyl, alkenyl,
     etc.; R3 = CON(R1)LQ2Q3R7, N(R1)COLQ2Q3R7, etc.; L = bond, alkyl, alkenyl,
     etc.; Q2, Q3 = bond, alkyl, alkenyl, etc.; R7 = H, alkyl, alkenyl, etc.]
     and their pharmaceutically acceptable salts and formulations were prepared
     For example, coupling of chloropyrimidine II and 7-amino-2,3-
     dihydroisoindol-1-one afforded diaminophenylpyrimidine III in 33% yield.
     Compds. I are claimed to be useful for the treatment of diseases
     characterized by excessive or anomalous cell proliferation.
ACCESSION NUMBER:        2006:194015  HCAPLUS
DOCUMENT NUMBER:         144:292768
TITLE:                   Preparation of 2,4-di(aminophenyl)pyrimides as protein
                         PLK1 inhibitors
INVENTOR(S):             Stadtmueller, Heinz; Engelhardt, Harald; Steegmaier,
                         Martin; Baum, Anke; Guertler, Ulrich; Schoop, Andreas;
                         Quant, Jens; Solca, Flavio; Hauptmann, Rudolf; Reiser,
                         Ulrich; Zahn, Stephan Karl; Herfurth, Lars
PATENT ASSIGNEE(S):      Boehringer Ingelheim International G.m.b.H., Germany
SOURCE:                  PCT Int. Appl., 272 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                German
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND    DATE        APPLICATION NO.         DATE
     ---------------     ----    --------    --------------------    --------
     WO 2006021544        A1     20060302    WO 2005-EP54089         20050818
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
             SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
L4   ANSWER 4 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)
               ZA, ZM, ZW
           RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
               IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
               CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
               GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
               KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.:                      EP 2004-19775       A  20040820
IT   878153-62-9P 878153-63-0P 878153-64-1P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of 2,4-di(aminophenyl)pyrimides as protein PLK1 inhibitors)
RN   878153-62-9  HCAPLUS
CN   Benzamide, 4-[[4-[[2-(2-fluoroethyl)-2,3-dihydro-1-methyl-3-oxo-1H-
     isoindol-4-yl]amino]-5-nitro-2-pyrimidinyl]amino]-3-methoxy-N-[trans-4-(4-
     morpholinyl)cyclohexyl]- (9CI)   (CA INDEX NAME)

Relative stereochemistry.

                                                 PAGE 1-A
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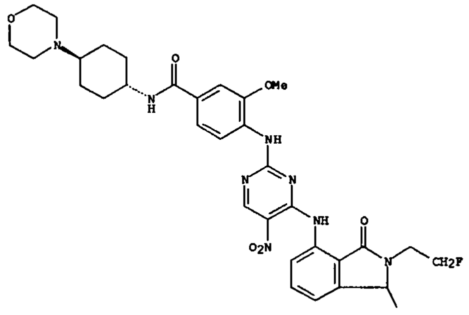

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                                                 PAGE 2-A
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RN   878153-63-0  HCAPLUS
CN   Benzamide, 4-[[4-[[2-(2-fluoroethyl)-2,3-dihydro-1-methyl-3-oxo-1H-
     isoindol-4-yl]amino]-5-nitro-2-pyrimidinyl]amino]-3-methoxy-N-(1-methyl-4-
     piperidinyl)- (9CI)   (CA INDEX NAME)
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L4   ANSWER 4 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)
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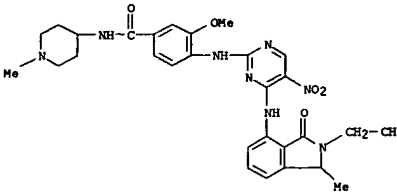

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RN   878153-64-1  HCAPLUS
CN   Benzamide, 4-[[4-[[2-(2-fluoroethyl)-2,3-dihydro-1-methyl-3-oxo-1H-
     isoindol-4-yl]amino]-5-nitro-2-pyrimidinyl]amino]-3-methoxy-N-[2-(1-
     pyrrolidinyl)ethyl]- (9CI)   (CA INDEX NAME)
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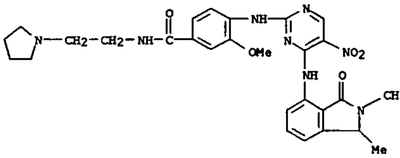

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REFERENCE COUNT:        4      THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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L4   ANSWER 5 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  03 Mar 2006
GI


* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

AB   Title compds. I [Z = LQ1Q2R4; X = N, CRe with provisos; Y = N, CH; R1 = H,
     halo, =O, etc.; R2 = H, alkyl, alkenyl, etc.; R3 = H, halo, OR5, etc.; L =
     bond, alkyl, alkenyl, etc.; Q1, Q2 = bond, alkyl, alkenyl, etc.; R4 = H,
     alkyl, alkenyl, etc.; Ra, Rb, Rc = H, halo, NO2, etc.; R5 = H, alkyl,
     alkenyl, etc.] and their pharmaceutically acceptable salts and
     formulations were prepared  For example, coupling of benzoic acid II and
     trans-4-morpholin-4-ylcyclohexylamine afforded, after work-up, the formate
     salt of pteridinediol III in 51% yield.  Compds. I are claimed to be
     useful as protein PLK1 inhibitors (no data provided).
ACCESSION NUMBER:        2006:193918  HCAPLUS
DOCUMENT NUMBER:         144:274293
TITLE:                   Preparation of 2-amino-6,7-pteridinediol and related
                         compounds as protein PLK1 inhibitors
INVENTOR(S):             Stadtmueller, Heinz; Engelhardt, Harald; Schoop,
                         Andreas; Steegmaier, Martin
PATENT ASSIGNEE(S):      Boehringer Ingelheim International G.m.b.H., Germany
SOURCE:                  PCT Int. Appl., 66 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                German
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
     ---------------     ----   --------    --------------------    --------
     WO 2006021547        A1    20060302    WO 2005-EP54096         20050819
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
             SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
             ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     US 2006047118        A1    20060302    US 2005-211048          20050824
PRIORITY APPLN. INFO.:                      EP 2004-20291       A  20040826
IT   877661-65-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of aminopteridinediol and related compds. as protein PLK1
        inhibitors)
RN   877661-65-9  HCAPLUS
CN   Benzoic acid, 4-[[4-(cyclopentylamino)-5-nitro-2-pyrimidinyl]amino]-3-
     methoxy-, phenylmethyl ester (9CI)   (CA INDEX NAME)
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L4   ANSWER 5 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)
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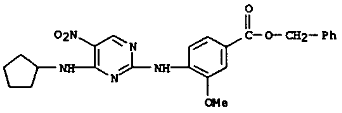

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REFERENCE COUNT:        3      THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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L4 ANSWER 6 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 26 Jan 2006
AB The present invention relates to the use of compds. capable of inhibiting protein aggregate formation and capable of depolymg. protein aggregates for the preparation of a pharmaceutical composition for treating neurodegenerative conditions such as Alzheimer disease.

ACCESSION NUMBER: 2006:74852 HCAPLUS
DOCUMENT NUMBER: 144:164276
TITLE: Treating neurodegenerative conditions
INVENTOR(S): Mandelkow, Eckard; Mandelkow, Eva-Maria; Biernat, Jacek; Bergen, Martin V.; Pickhardt, Markus
PATENT ASSIGNEE(S): Max Planck Gesellschaft zur Foerderung der Wissenschaft, Germany
SOURCE: PCT Int. Appl., 136 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
     ---------------     ----   --------    --------------------    --------
     WO 2006007864        A1    20060126    WO 2004-EP8031          20040717
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI,
             CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS,
             MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD,
             RU, TJ, TM
PRIORITY APPLN. INFO.:                          WO 2004-EP8031          20040717
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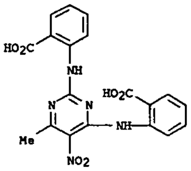
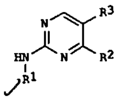
OTHER SOURCE(S): MARPAT 144:164276
IT **300719-17-9**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compds. to treat neurodegenerative conditions)
RN 300719-17-9 HCAPLUS
CN Benzoic acid, 2,2'-[(6-methyl-5-nitro-2,4-pyrimidinediyl)diimino]bis- (9CI) (CA INDEX NAME)



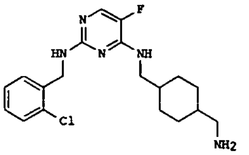
L4 ANSWER 6 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 10 Jun 2005
GI



I

R2 = hXY



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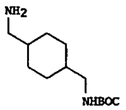

III

AB Title compds. I [wherein R1 = (un)substituted heteroaryl/aryl/cyclo/cycloalkyl/alkyl, naphthyl, quinolinyl, etc.; R2 = (un)substituted -NH-CH2-(CH2)n-CH2-NR4R5, -NH-(CH2)p-phenylene-(CH2)q-NR4R5, -NH(CH2)p-X-R4, etc.; X = piperidinyl; n = 3-8; p = 1-3; q = 0-3; R4, R5 = independently H, amidino, (un)substituted aryl/alkyl; R3 = halo, CN, NO2, aminocarbonyl, (un)substituted alkyl, alkyloxycarbonyl; their tautomers, pharmaceutically acceptable salts, solvates, or amino-protected derivs., with certain compds. excluded] were prepared as inhibitors of protein kinase C (PKC)-theta useful for treating immunol. disorders and type II diabetes. For example, II was prepared in 5 steps via amination of 2,4-dichloro-5-fluoropyrimidine with amine III and 2-chlorobenzylamine. Selected I inhibited PKC-theta with IC50 values ≤ 0.3 μM. Thus, I are useful for treating a disease or disorder associated with T cells activation.

ACCESSION NUMBER: 2005:497492 HCAPLUS
DOCUMENT NUMBER: 143:7727
TITLE: Preparation of 2,4-diaminopyrimidine derivatives as inhibitors of PKC-theta for treating diseases associated with T cells activation, in particular immunol. disorders and type II diabetes
INVENTOR(S): Cardozo, Mario G.; Cogan, Derek; Cywin, Charles Lawrence; Dahmann, George; Disalvo, Darren; Ginn, John David; Prokopowicz, Anthony S.; Spero, Denice M.; Young, Erick ~~Richard Roush~~
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA; Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G.
SOURCE: U.S. Pat. Appl. Publ., 69 pp., Cont.-in-part of U.S. Ser. No. 766,079.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

L4 ANSWER 7 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
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     US 2005124640        A1    20050609    US 2004-933635          20040903
     US 2004242613        A1    20041202    US 2004-766079          20040127
PRIORITY APPLN. INFO.:                      US 2003-443700P      P  20030130
                                            US 2004-766079       A2 20040127
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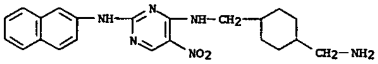
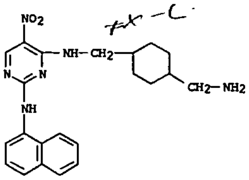
OTHER SOURCE(S): MARPAT 143:7727
IT **736051-05-1P 736051-54-0P 736052-41-8P 736052-46-3P 736052-50-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(PKC-theta inhibitor; preparation of diaminopyrimidines as PKC-theta inhibitors for treating diseases associated with T cells activation, in particular immunol. disorders and type II diabetes)
RN 736051-05-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)cyclohexyl]methyl]-N2-2-naphthalenyl-5-nitro- (9CI) (CA INDEX NAME)

Fx-L



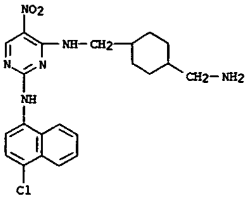
RN 736051-54-0 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)cyclohexyl]methyl]-N2-1-naphthalenyl-5-nitro- (9CI) (CA INDEX NAME)

Fx-L

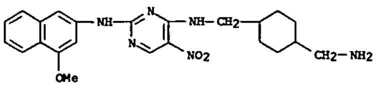


RN 736052-41-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)cyclohexyl]methyl]-N2-(4-chloro-1-naphthalenyl)-5-nitro- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 736052-46-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)cyclohexyl]methyl]-N2-(4-methoxy-2-naphthalenyl)-5-nitro- (9CI) (CA INDEX NAME)



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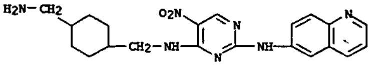
RN 736052-50-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)cyclohexyl]methyl]-5-nitro-N2-6-quinolinyl- (9CI) (CA INDEX NAME)



L4 ANSWER 8 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 27 May 2005

AB Compns. and methods using substituted pyrimidines are provided. The substituted pyrimidines may be used to treat diseases modulated by NGFI-B family activity.

ACCESSION NUMBER: 2005:451367 HCAPLUS
DOCUMENT NUMBER: 142:476293
TITLE: Substituted pyrimidine compositions and methods using them for the treatment of NGFI-B-related diseases
INVENTOR(S): Martin, Richard; Mohan, Raju; Ordentlich, Peter
PATENT ASSIGNEE(S): X-Ceptor Therapeutics, Inc., USA
SOURCE: PCT Int. Appl., 117 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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     PATENT NO.          KIND    DATE      APPLICATION NO.       DATE
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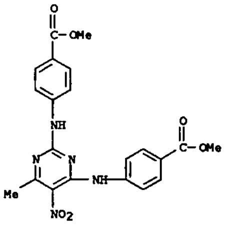
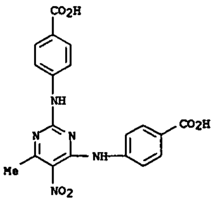
     WO 2005047268        A2     20050526  WO 2004-US37642       20041109
     WO 2005047268        A3     20050721
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO,
             SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
PRIORITY APPLN. INFO.:                     US 2003-519030P     P  20031110
```

OTHER SOURCE(S): MARPAT 142:476293
IT **312499-77-7 331971-30-3**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pyrimidine derivs. for treatment of NGFI-B-related diseases)
RN 312499-77-7 HCAPLUS
CN Benzoic acid, 4,4'-[(6-methyl-5-nitro-2,4-pyrimidinediyl)diimino]bis-, dimethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 8 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



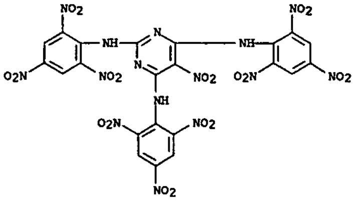
RN 331971-30-3 HCAPLUS
CN Benzoic acid, 4,4'-[(6-methyl-5-nitro-2,4-pyrimidinediyl)diimino]bis- (9CI) (CA INDEX NAME)



L4 ANSWER 9 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 02 May 2005

AB Neural network (NN) studies were used to predict impact sensitivity of various explosive mols. A total of 234 explosive mols. were taken from a single database and 39 mol. descriptors were computed for each explosive mol. Optimization of NN architecture was done by examining 7 sets of mol. descriptors and varying the number of hidden neurons. To optimize NN architecture, 17 mol. descriptors were used, composed of compositional and topol. descriptors in an input layer, and 2 hidden neurons in a hidden layer.

ACCESSION NUMBER: 2005:372122 HCAPLUS
DOCUMENT NUMBER: 144:26320
TITLE: Optimization of neural networks architecture for impact sensitivity of energetic molecules
AUTHOR(S): Cho, Soo Gyeong; No, Kyoung Tai; Goh, Eun Mee; Kim, Jeong Kook; Shin, Jae Hong; Joo, Young Dae; Seong, Seeyearl
CORPORATE SOURCE: Agency for Defense Development, Daejeon, 305-600, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (2005), 26(3), 399-408
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **41230-78-8**
RL: PRP (Properties)
(occupational safety in relation to optimized neural network architecture to assess energetic mol. impact sensitivity)
RN 41230-78-8 HCAPLUS
CN 2,4,6-Pyrimidinetriamine, 5-nitro-N,N',N''-tris(2,4,6-trinitrophenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 15 Apr 2005

AB The invention provides methods relating to a novel screening assay format that can be applied to broad members of the protein kinase gene family. More specifically, the assay was used for inhibitors of STK12 kinase domain. The assay uses a series of fluorescently labeled, active site probes described herein that can be displaced by an inhibitor agent. The Kd for the inhibitor compound is derived based on the Kd of the probe for the kinase and the dose response of the inhibitor agent. The invention also provides novel active site probes suitable for use with the screening method.

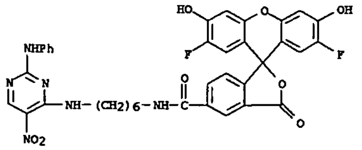
ACCESSION NUMBER: 2005:324323 HCAPLUS
DOCUMENT NUMBER: 142:367631
TITLE: Fluorescent probes for use in protein kinase inhibitor binding competition assay for screening applications
INVENTOR(S): Prokopowicz, Anthony S.; Brown, Martha Priscilla; Wildeson, Jessi Marie; Jakes, Scott; Labadia, Mark E.
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Appl

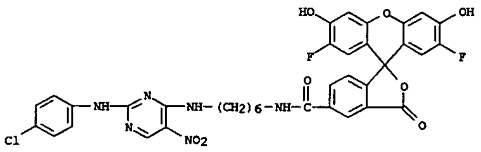
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005033330	A2	20050414	WO 2004-US32253	20040930
WO 2005033330	A3	20050728		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005100978	A1	20050512	US 2004-955129	20040930
PRIORITY APPLN. INFO.:			US 2003-508539P P	20031003

OTHER SOURCE(S): MARPAT 142:367631
IT **849339-53-3 849339-54-4 849339-55-5 849339-56-6 849339-57-7**
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(fluorescent probe; fluorescent probes for use in protein kinase inhibitor binding competition assay for screening applications)
RN 849339-53-3 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxamide, 2',7'-difluoro-3',6'-dihydroxy-N-[6-[[5-nitro-2-(phenylamino)-4-pyrimidinyl]amino]hexyl]-3-oxo- (9CI) (CA INDEX NAME)

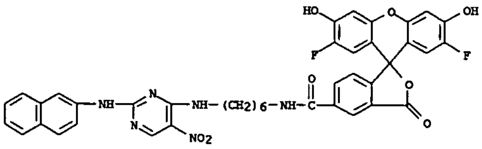
L4 ANSWER 10 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 849339-54-4 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxamide, N-[6-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]hexyl]-2',7'-difluoro-3',6'-dihydroxy-3-oxo- (9CI) (CA INDEX NAME)

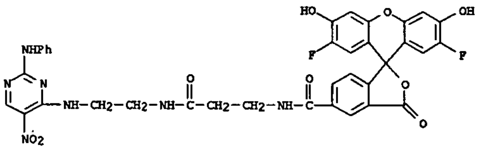


RN 849339-55-5 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxamide, 2',7'-difluoro-3',6'-dihydroxy-N-[6-[[2-(2-naphthalenylamino)-5-nitro-4-pyrimidinyl]amino]hexyl]-3-oxo- (9CI) (CA INDEX NAME)

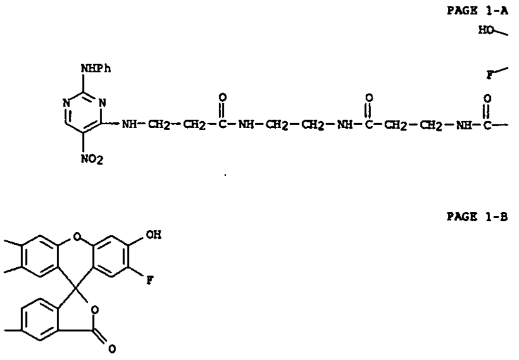


RN 849339-56-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxamide, 2',7'-difluoro-3',6'-dihydroxy-N-[3-[[2-[[5-nitro-2-(phenylamino)-4-pyrimidinyl]amino]ethyl]amino]-3-oxopropyl]-3-oxo- (9CI) (CA INDEX NAME)

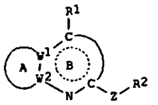
L4 ANSWER 10 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 849339-57-7 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxamide, 2',7'-difluoro-3',6'-dihydroxy-N-[3-[[2-[[3-[[5-nitro-2-(phenylamino)-4-pyrimidinyl]amino]-1-oxopropyl]amino]ethyl]amino]-3-oxopropyl]-3-oxo- (9CI) (CA INDEX NAME)



L4 ANSWER 11 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 25 Mar 2005
GI



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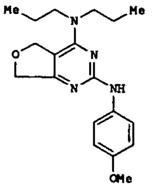

II

AB Title compds. I [ring A = optionally substituted monocycle with (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, etc.; ring B = monocyclic unsatd. heterocycle which may addnl. contain one or two N, O, optionally oxidized sulfur; W1, W2 = C, N; Z = NR3, O, optionally oxidized sulfur, etc.; R3 = H, (un)substituted alkyl, (un)substituted alkenyl, etc.; R1 = (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl etc.; R2 = (un)substituted unsatd. cyclic group] were prepared For example, aromatic nucleophilic substitution of 2-chloro-4-(N,N-di-n-propylamino)-5,7-dihydrofuro[3,4-d]pyrimidine, e.g., prepared from 4-ocotetrahydrofuran-3-carboxylic acid Me ester in 3 steps, with 2-chloro-4-methoxyaniline afforded compound II. In CRF (corticotropin-releasing factor) binding assays, compds. I exhibited the IC50 values of <1 μM. Compds. I are claimed useful for the treatment of neuropsychiatric diseases, digestive diseases. Formulations are given.

ACCESSION NUMBER: 2005:260031 HCAPLUS
DOCUMENT NUMBER: 142:336397
TITLE: Preparation of fused pyrimidine and related compounds as CRF antagonists
INVENTOR(S): Nakai, Hisao; Saito, Tetsuji; Obitsu, Tetsuo; Minamoto, Chiaki; Yoshida, Mayuki; Kishi, Akihiro; Katsumata, Seishi; Katayama, Hideo
PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 163 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005026126	A1	20050324	WO 2004-JP13386	20040908
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,				

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L4   ANSWER 11 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)
             SN, TD, TG
PRIORITY APPLN. INFO.:                       JP 2003-316662      A  20030909
                                             JP 2004-122409      A  20040419
OTHER SOURCE(S):           MARPAT 142:336397
IT   848398-83-4P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of fused pyrimidines as CRF antagonists for treatment of
        neuropsychiatric diseases, digestive diseases)
RN   848398-83-4  HCAPLUS
CN   2,4,6-Pyrimidinetriamine, N2-(2-chloro-4-methoxyphenyl)-N2-methyl-5-nitro-
     N4,N4-dipropyl- (9CI)  (CA INDEX NAME)
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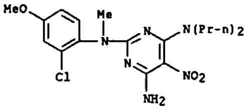

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REFERENCE COUNT:           23    THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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L4   ANSWER 12 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  24 Feb 2005
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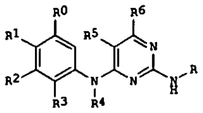

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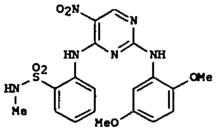

II

```
AB   The title compds. I [R = aryl, heteroaryl, cycloalkyl and
     heterocycloalkyl; R0-R3 = H, alkyl, cycloalkyl, etc.; R4 = H, alkyl; R5,
     R6 = H, alkyl, alkoxyalkyl, etc.], useful for the manufacture of a medicament
     for the treatment or prevention of a disease which responds to inhibition
     of FAK and/or ALK and/or ZAP-70 and/or IGF-IR, were prepared and formulated.
     E.g., a 2-step synthesis of II, starting from 2,4-dichloro-5-
     nitropyrimidine and 2-amino-N-methylbenzenesulfonamide, was given.  The
     compds. I have IC50 values in the range of 10 nM to 2 µM in cell-free
     ZAP-70 kinase assay.
ACCESSION NUMBER:        2005:158647  HCAPLUS
DOCUMENT NUMBER:         142:261547
TITLE:                   Preparation of 2,4-pyrimidinediamines useful in the
                         treatment of neoplastic diseases, inflammatory and
                         immune system disorders
INVENTOR(S):             Garcia-echeverria, Carlos; Kanazawa, Takanori;
                         Kawahara, Eiji; Masuya, Keiichi; Matsuura, Naoko;
                         Miyake, Takahiro; Ohmori, Osamu; Umemura, Ichiro;
                         Steensma, Ruo; Chopiuk, Greg; Jiang, Jiqing; Wan,
                         Yongqin; Ding, Qiang; Zhang, Qiong; Gray, Nathanael
                         Schiander; Karanewsky, Donald
PATENT ASSIGNEE(S):      Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.; IRM
                         LLC
SOURCE:                  PCT Int. Appl., 285 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                English
FAMILY ACC. NUM. COUNT:  2
PATENT INFORMATION:
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L4   ANSWER 12 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)

     PATENT NO.          KIND   DATE       APPLICATION NO.         DATE
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     WO 2005016894        A1    20050224   WO 2004-EP9099          20040813
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
     AU 2004264382        A1    20050224   AU 2004-264382          20040813
     CA 2533320           AA    20060224   CA 2004-2533320         20040813
PRIORITY APPLN. INFO.:                     GB 2003-19227        A  20030815
                                           GB 2003-22370        A  20030924
                                           WO 2004-EP9099       W  20040813
OTHER SOURCE(S):           MARPAT 142:261547
IT   761436-42-4P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of 2,4-pyrimidinediamines useful in the treatment of neoplastic
        diseases, inflammatory and immune system disorders)
RN   761436-42-4  HCAPLUS
CN   Benzenesulfonamide, 2-[[2-[(2,5-dimethoxyphenyl)amino]-5-nitro-4-
     pyrimidinyl]amino]-N-methyl- (9CI)  (CA INDEX NAME)
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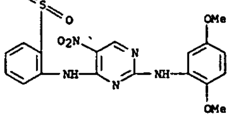

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REFERENCE COUNT:           19    THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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L4   ANSWER 13 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  11 Feb 2005
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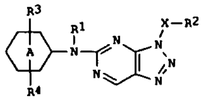

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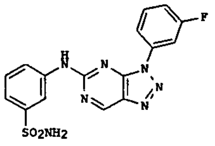

II

```
AB   The title compds. I [ring A = Ph, pyridyl, pyrimidinyl, pyridazinyl or
     pyrazinyl; R1 = H, aryl, formyl, etc.; X = a direct bond, (CH2)n or
     (CH2)mX1aX1b (n = 1-4; m = 1-2; X1a = O, C(O), NR5; X1b = a direct bond,
     alkyl); R2 = cycloalkyl, Ph, 4-7 membered monocyclic heterocycle containing at
     least one heteroatom. selected from O, S or N, benzoxazolyl, etc.; R3 =
     halo, OH, (un)substituted alkyl, alkenyl or alkynyl, etc.; R4 = H, halo,
     OH, (un)substituted alkyl, etc.; R5 = H, alkyl, alkenyl], useful for the
     prevention or the treatment of diseases mediated through GSK3, were prepared
     E.g., a 4-step synthesis of II which showed pIC50 of > 8 against
     GSK3β and against GSK3α, was given.  The pharmaceutical composition
     comprising the compound I is disclosed.
ACCESSION NUMBER:        2005:122890  HCAPLUS
DOCUMENT NUMBER:         142:219305
TITLE:                   Preparation of triazolopyrimidines as glycogen
                         synthase kinase 3 inhibitors
INVENTOR(S):             Freyne, Eddy Jean Edgard; Love, Christopher John;
                         Cooymans, Ludwig Paul; Vandermaesen, Nele; Buijnsters,
                         Peter Jacobus Johannes Antonius; Willems, Marc;
                         Embrechts, Werner Constant Johan
PATENT ASSIGNEE(S):      Janssen Pharmaceutica N.V., Belg.
SOURCE:                  PCT Int. Appl., 124 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                English
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE       APPLICATION NO.         DATE
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     WO 2005012307        A1    20050210   WO 2004-EP51455         20040712
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
L4   ANSWER 13 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)
              LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
              TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
          RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
              AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
              EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
              SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
              SN, TD, TG
     AU 2004260738          A1     20050210    AU 2004-260738          20040712
     CA 2531333             AA     20050210    CA 2004-2531333         20040712
PRIORITY APPLN. INFO.:                         WO 2003-EP50310      A  20030716
                                               WO 2003-EP350310     A  20030716
                                               WO 2004-EP51455      W  20040712
OTHER SOURCE(S):          MARPAT 142:219305
IT   521304-07-4P 840537-59-9P 840537-60-2P
     840537-61-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of triazolopyrimidines as glycogen synthase kinase 3
        inhibitors)
RN   521304-07-4  HCAPLUS
CN   Benzamide, 3-[[5-nitro-4-[(phenylmethyl)amino]-2-pyrimidinyl]amino]- (9CI)
       (CA INDEX NAME)
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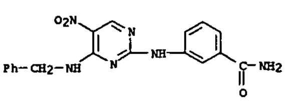

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RN   840537-59-9  HCAPLUS
CN   Benzonitrile, 3-[[4-[(3,5-dimethoxyphenyl)amino]-5-nitro-2-
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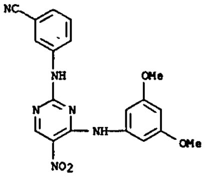

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RN   840537-60-2  HCAPLUS
CN   Benzenesulfonamide, 4-[[5-nitro-4-(phenylamino)-2-pyrimidinyl]amino]-
     (9CI)  (CA INDEX NAME)
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L4   ANSWER 13 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)
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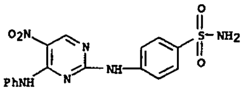

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RN   840537-61-3  HCAPLUS
CN   Benzamide, 3,3'-[(5-nitro-2,4-pyrimidinediyl)diimino]bis- (9CI)  (CA INDEX
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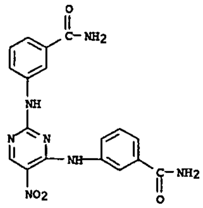

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REFERENCE COUNT:          4       THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
                                  RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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L4   ANSWER 14 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  11 Feb 2005
GI
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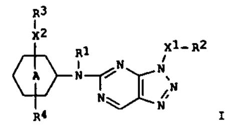

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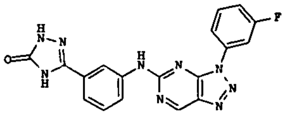

II

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AB   The title compds. I [ring A = Ph, pyridyl, pyrimidinyl, pyridazinyl or
     pyrazinyl; R1 = H, aryl, formyl, etc.; X = a direct bond, (CH2)n or
     (CH2)mX1aX1b (n = 1-4; m = 1-2; X1a = O, C(O), NR5; X1b = a direct bond,
     alkyl); R2 = cycloalkyl, Ph, 4-7 membered monocyclic heterocycle containing at
     least one heteroatom. selected from O, S or N, benzoxazolyl, etc.; X2 = a
     direct bond, O, C(O), etc.; R3 = (un)substituted 5-6 membered monocyclic
     heterocyclyl or 9-10 membered bicyclic heterocyclyl, etc.; R4 = H, halo,
     OH, (un)substituted alkyl, etc.; R5 = H, alkyl, alkenyl], useful for the
     prevention or the treatment of diseases mediated through GSK3, were prepared
     E.g., a 4-step synthesis of II which showed pIC50 of > 8 against
     GSK3β and against GSK3α, was given.  The pharmaceutical composition
     comprising the compound I is disclosed.
ACCESSION NUMBER:         2005:122889  HCAPLUS
DOCUMENT NUMBER:          142:219304
TITLE:                    Preparation of triazolopyrimidines as glycogen
                          synthase kinase 3 inhibitors
INVENTOR(S):              Freyne, Eddy Jean Edgard; Love, Christopher John;
                          Cooymans, Ludwig Paul; Vandermaesen, Nele; Buijnsters,
                          Peter Jacobus Johannes Antonius; Willems, Marc;
                          Embrechts, Werner Constant Johan
PATENT ASSIGNEE(S):       Janssen Pharmaceutica N.V., Belg.
SOURCE:                   PCT Int. Appl., 109 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

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     WO 2005012304        A2    20050210   WO 2004-EP51457         20040712
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
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L4   ANSWER 14 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)
              LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
              TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
          RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
              AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
              EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
              SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
              SN, TD, TG
     AU 2004260739          A1     20050210    AU 2004-260739          20040712
     CA 2531232             AA     20050210    CA 2004-2531232         20040712
PRIORITY APPLN. INFO.:                         WO 2003-EP350314     A  20030716
                                               WO 2004-EP51457      W  20040712
OTHER SOURCE(S):          MARPAT 142:219304
IT   842129-23-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of triazolopyrimidines as glycogen synthase kinase 3
        inhibitors)
RN   842129-23-1  HCAPLUS
CN   2,4-Pyrimidinediamine, N2-[4-(4-methyl-1-piperazinyl)phenyl]-5-nitro-N4-
     phenyl- (9CI)  (CA INDEX NAME)
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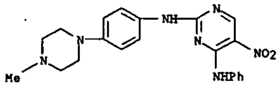

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IT   842129-16-2P 842129-17-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of triazolopyrimidines as glycogen synthase kinase 3
        inhibitors)
RN   842129-16-2  HCAPLUS
CN   2,4-Pyrimidinediamine, N4-cyclohexyl-N2-[4-(4-morpholinyl)phenyl]-5-nitro-
     (9CI)  (CA INDEX NAME)
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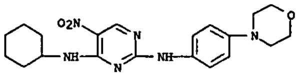

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RN   842129-17-3  HCAPLUS
CN   2,4-Pyrimidinediamine, N4-cyclohexyl-N2-[4-(4-methyl-1-piperazinyl)phenyl]-
     5-nitro- (9CI)  (CA INDEX NAME)
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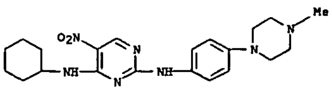

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L4   ANSWER 15 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  24 Sep 2004
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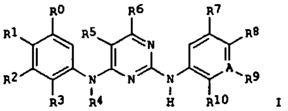

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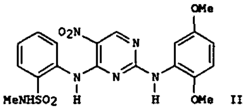

II

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AB   The title pyrimidine derivs. I [R0-R3 = H, alkyl, aryl, etc.; or R0 and
     R1, R1 and R2, and/or R2 and R3 form, together with the carbon atoms to
     which they are attached, 5-6 membered carbocyclic or heterocyclic ring
     comprising 0-3 heteroatoms selected from N, O and S; R4 = H, alkyl; R5, R6
     = H, alkyl, alkoxyalkyl, halo, etc.; R7-R10 = alkyl, cycloalkyl, aryl,
     etc.; or R7 and R8, R8 and R9, and/or R9 and R10 form, together with the
     carbon atoms to which they are attached, 5-6 membered carbocyclic or
     heterocyclic ring comprising 0-3 heteroatoms selected from N, O and S; A =
     C, N], useful as FAK or/and IGF-1 receptor inhibitors in the treatment of
     neoplastic diseases, inflammatory and immune system disorders, were prepared
     and formulated.  E.g., a 2-step synthesis of II from 2,4-dichloro-5-
     nitropyrimidine, 2-amino-N-methylbenzenesulfonamide, and
     2,5-dimethoxyaniline which showed IC50 of 140 nM in FAK assay, was given.
     The pharmaceutical composition comprising the compound I is claimed.
ACCESSION NUMBER:         2004:780679  HCAPLUS
DOCUMENT NUMBER:          141:296041
TITLE:                    Preparation of novel 2,4-di(phenylamino)pyrimidines
                          useful in the treatment of neoplastic diseases,
                          inflammatory and immune system disorders
INVENTOR(S):              Garcia-Echeverria, Carlos; Kanazawa, Takanori;
                          Kawahara, Eiji; Masuya, Keiichi; Matsuura, Naoko;
                          Miyake, Takahiro; Ohmori, Osamu; Umemura, Ichiro
PATENT ASSIGNEE(S):       Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
SOURCE:                   PCT Int. Appl., 185 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   2
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
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L4   ANSWER 15 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
             SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
             TD, TG
     AU 2004220338        A1    20040923    AU 2004-220338          20040312
     CA 2518932           AA    20040923    CA 2004-2518932         20040312
     EP 1606265           A1    20051221    EP 2004-719989          20040312
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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     BR 2004008347        A     20060321    BR 2004-8347            20040312
PRIORITY APPLN. INFO.:                      GB 2003-5929         A  20030314
                                            GB 2003-19227        A  20030815
                                            GB 2003-22370        A  20030924
                                            WO 2004-EP2616       A  20040312
OTHER SOURCE(S):          MARPAT 141:296041
IT   761436-42-4P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of 2,4-di(phenylamino)pyrimidines as FAK or/and IGF-1 receptor
        inhibitors useful in the treatment of neoplastic diseases, inflammatory
        and immune system disorders)
RN   761436-42-4  HCAPLUS
CN   Benzenesulfonamide, 2-[[2-[(2,5-dimethoxyphenyl)amino]-5-nitro-4-
     pyrimidinyl]amino]-N-methyl- (9CI)  (CA INDEX NAME)
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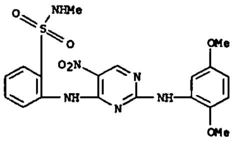

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REFERENCE COUNT:          10     THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
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ED   Entered STN:  02 Sep 2004
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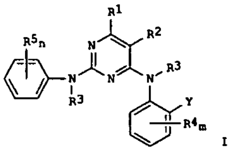

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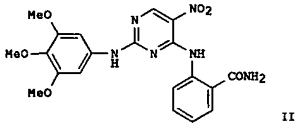

II

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AB   Title compds. represented by the formula I [wherein R1 = H, halo, alkyl,
     alkenyl, alkynyl; R2 = halo, (cyclo)alkyl, (cyclo)alkenyl, alkynyl, etc.;
     R3 = independently H or alkyl; R4 = independently halo, (cyclo)alkyl,
     (cyclo)alkenyl, NO2, etc.; R5 = independently alkyl, alkenyl, amino, etc.;
     Y = carbonylalkyl, amino, sulfonyl, etc.; m = 0-3; n = 0-5; and
     pharmaceutically acceptable salts, solvates or physiol. functional derivs.
     thereof] were prepared as Polo-like kinases (PLK) inhibitors.  For example,
     reaction of 2-[(2-chloro-5-nitropyrimidin-4-yl)amino]benzamide with
     3,4,5-trimethoxyaniline gave II•HCl in 35% yield.  I were tested for
     inhibition of PLK1 and methylene blue growth.  Thus, I and their
     pharmaceutical compns. are useful for the treatment of PLK-mediated
     conditions and a susceptible neoplasm, such as breast cancer, colon
     cancer, lung cancer, prostate cancer, lymphoma, leukemia, endometrial
     cancer, melanoma,ovarian cancer, pancreatic cancer, squamous carcinoma,
     carcinoma of the head and neck, and esophageal carcinoma (no data).
ACCESSION NUMBER:         2004:718507  HCAPLUS
DOCUMENT NUMBER:          141:243557
TITLE:                    Preparation of pyrimidine derivatives as Polo-like
                          kinases inhibitors for treatment of cancers
INVENTOR(S):              Davis-Ward, Ronda; Mook, Robert Anthony, Jr.; Neeb,
                          Michael J.; Salovich, James M.
PATENT ASSIGNEE(S):       SmithKline Beecham Corporation, USA
SOURCE:                   PCT Int. Appl., 115 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
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     WO 2004074244        A2    20040902    WO 2004-US4197          20040211
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L4   ANSWER 16 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE,
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     EP 1597251           A2    20051123    EP 2004-710264          20040211
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PRIORITY APPLN. INFO.:                      US 2003-448795P      P  20030220
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OTHER SOURCE(S):          MARPAT 141:243557
IT   748797-67-3P 748797-69-5P 748797-71-9P
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     748797-81-1P 748797-83-3P 748797-84-4P
     748797-86-6P 748797-88-8P 748797-90-2P
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     748798-09-6P 748798-11-0P 748798-13-2P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of pyrimidine derivs. as Polo-like kinases inhibitors for
        treatment of cancers)
RN   748797-67-3  HCAPLUS
CN   Benzoic acid, 2-[[5-nitro-2-[(3,4,5-trimethoxyphenyl)amino]-4-
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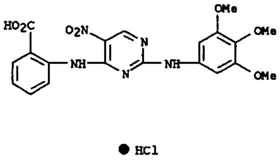

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RN   748797-69-5  HCAPLUS
CN   Benzamide, 2-[[5-nitro-2-[(3,4,5-trimethoxyphenyl)amino]-4-
     pyrimidinyl]amino]-, monohydrochloride (9CI)  (CA INDEX NAME)
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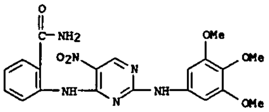
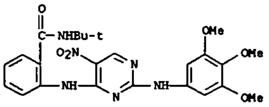


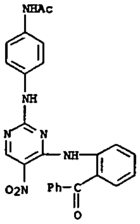
● HCl

RN 748797-71-9 HCAPLUS
CN Benzamide, N-(1,1-dimethylethyl)-2-[[5-nitro-2-[(3,4,5-trimethoxyphenyl)amino]-4-pyrimidinyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)



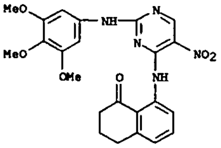
● HCl

RN 748797-73-1 HCAPLUS
CN Acetamide, N-[4-[[4-[(2-benzoylphenyl)amino]-5-nitro-2-pyrimidinyl]amino]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



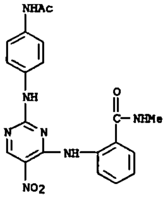
● HCl

RN 748797-75-3 HCAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-8-[[5-nitro-2-[(3,4,5-trimethoxyphenyl)amino]-4-pyrimidinyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)



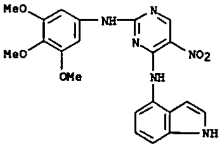
● HCl

RN 748797-79-7 HCAPLUS
CN Benzamide, 2-[[2-[[4-(acetylamino)phenyl]amino]-5-nitro-4-pyrimidinyl]amino]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



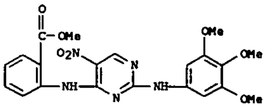
● HCl

RN 748797-81-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-1H-indol-4-yl-5-nitro-N2-(3,4,5-trimethoxyphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



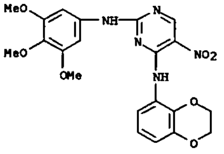
● HCl

RN 748797-83-3 HCAPLUS
CN Benzoic acid, 2-[[5-nitro-2-[(3,4,5-trimethoxyphenyl)amino]-4-pyrimidinyl]amino]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



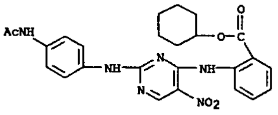
● HCl

RN 748797-84-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-(2,3-dihydro-1,4-benzodioxin-5-yl)-5-nitro-N2-(3,4,5-trimethoxyphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



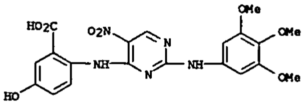
● HCl

RN 748797-86-6 HCAPLUS
CN Benzoic acid, 2-[[2-[[4-(acetylamino)phenyl]amino]-5-nitro-4-pyrimidinyl]amino]-, cyclohexyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

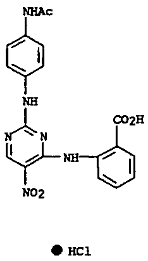
RN 748797-88-8 HCAPLUS
CN Benzoic acid, 5-hydroxy-2-[[5-nitro-2-[(3,4,5-trimethoxyphenyl)amino]-4-pyrimidinyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)



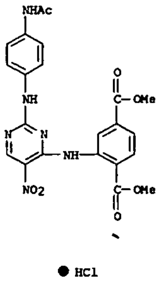
● HCl

RN 748797-90-2 HCAPLUS
CN Benzoic acid, 2-[[2-[[4-(acetylamino)phenyl]amino]-5-nitro-4-

pyrimidinyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)



RN 748797-97-9 HCAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-[[2-[[4-(acetylamino)phenyl]amino]-5-nitro-4-pyrimidinyl]amino]-, dimethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



RN 748797-99-1 HCAPLUS
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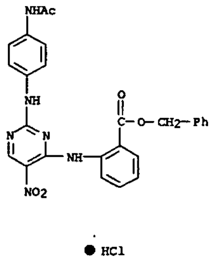
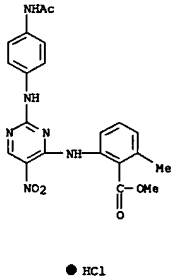
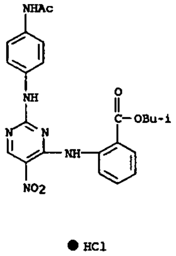


RN 748798-01-8 HCAPLUS
CN Benzoic acid, 2-[[2-[[4-(acetylamino)phenyl]amino]-5-nitro-4-pyrimidinyl]amino]-6-methyl-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



RN 748798-03-0 HCAPLUS
CN Benzoic acid, 2-[[2-[[4-(acetylamino)phenyl]amino]-5-nitro-4-pyrimidinyl]amino]-, 2-methylpropyl ester, monohydrochloride (9CI) (CA INDEX NAME)



RN 748798-05-2 HCAPLUS
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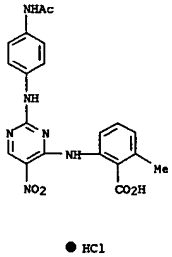
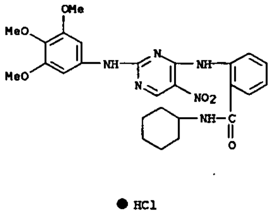
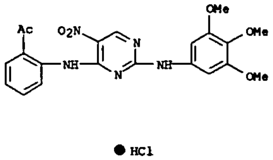


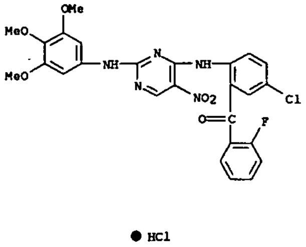
RN 748798-07-4 HCAPLUS
CN Benzamide, N-cyclohexyl-2-[[5-nitro-2-[(3,4,5-trimethoxyphenyl)amino]-4-pyrimidinyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)



RN 748798-09-6 HCAPLUS
CN Ethanone, 1-[2-[[5-nitro-2-[(3,4,5-trimethoxyphenyl)amino]-4-pyrimidinyl]amino]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

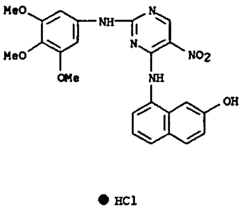


RN 748798-11-0 HCAPLUS
CN Methanone, [5-chloro-2-[[5-nitro-2-[(3,4,5-trimethoxyphenyl)amino]-4-pyrimidinyl]amino]phenyl](2-fluorophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



RN 748798-13-2 HCAPLUS

L4 ANSWER 16 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 2-Naphthalenol, 8-[[5-nitro-2-[(3,4,5-trimethoxyphenyl)amino]-4-pyrimidinyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)



L4 ANSWER 17 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 Aug 2004
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [wherein R1 = (un)substituted heteroaryl/aryl/cyclo/cycloalkyl/alkyl, naphthyl, quinolinyl, etc.; R2 = (un)substituted -NH-CH2-(CH2)n-CH2-NR4R5, -NH-(CH2)p-phenylene-(CH2)q-NR4R5, -NH(CH2)p-X-R4, etc.; X = pyridinyl; n = 3-8; p = 1-3; q = 0-3; R4, R5 = independently H, amidino, (un)substituted aryl/alkyl; R3 = halo, CN, NO2, aminocarbonyl, (un)substituted alkyl, alkyloxycarbonyl; their tautomers, pharmaceutically acceptable salts, solvates, or amino-protected derivs., with certain compds. excluded] were prepared as inhibitors of protein kinase C (PKC)-theta useful for treating immunol. disorders and type II diabetes. For example, II was prepared in 5 steps via amination of 2,4-dichloro-5-fluoropyrimidine with amine III and 2-chlorobenzylamine. Selected I inhibited PKC-theta with IC50 values ≤ 0.3 μM. Thus, I are useful for treating a disease or disorder associated with T cells activation.

ACCESSION NUMBER:	2004:648512 HCAPLUS
DOCUMENT NUMBER:	141:190795
TITLE:	Preparation of 2,4-diaminopyrimidine derivatives as inhibitors of PKC-theta for treating diseases associated with T cells activation, in particular immunol. disorders and type II diabetes
INVENTOR(S):	Cardozo, Mario G.; Cogan, Derek; Cywin, Charles Lawrence; Dahmann, Georg; Disalvo, Darren; Ginn, John David; Prokopowicz, Anthony S.; Spero, Denice M.; Young, Erick Richard Roush
PATENT ASSIGNEE(S):	Boehringer Ingelheim Pharmaceuticals, Inc., USA; Boehringer Ingelheim Pharma GmbH & Co. KG
SOURCE:	PCT Int. Appl., 124 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004067516	A1	20040812	WO 2004-US2240		20040127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI					
CA 2514612	AA	20040812	CA 2004-2514612		20040127
EP 1590334	A1	20051102	EP 2004-705675		20040127
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
PRIORITY APPLN. INFO.:			US 2003-443700P	P	20030130
			WO 2004-US2240	W	20040127

OTHER SOURCE(S): MARPAT 141:190795

IT **736051-05-1P**, N'-[[4-(Aminomethyl)cyclohexyl]methyl]-N-(2-naphthyl)-5-nitropyrimidine-2,4-diamine **736051-54-0P**, N'-[[4-(Aminomethyl)cyclohexyl]methyl]-N-(1-naphthyl)-5-nitropyrimidine-

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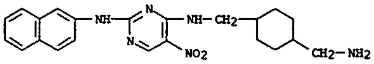
L4 ANSWER 17 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
2,4-diamine **736052-41-8P**, N'-[[4-(Aminomethyl)cyclohexyl]methyl]-N-(4-chloro-1-naphthyl)-5-nitropyrimidine-2,4-diamine **736052-46-3P**, N'-[[4-(Aminomethyl)cyclohexyl]methyl]-N-(4-methoxy-2-naphthyl)-5-nitropyrimidine-2,4-diamine **736052-50-9P**, N'-[[4-(Aminomethyl)cyclohexyl]methyl]-5-nitro-N-quinolin-6-ylpyrimidine-2,4-diamine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(PKC-theta inhibitor; prepn. of diaminopyrimidines as PKC-theta inhibitors for treating diseases assocd. with T cells activation, in particular immunol. disorders and type II diabetes)
RN 736051-05-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)cyclohexyl]methyl]-N2-2-naphthalenyl-5-nitro- (9CI) (CA INDEX NAME)



RN 736051-54-0 HCAPLUS
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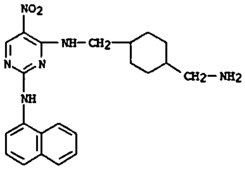

RN 736052-41-8 HCAPLUS
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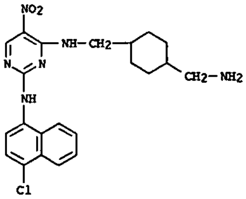
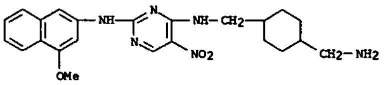
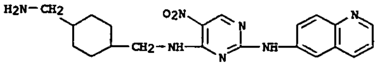


L4 ANSWER 17 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 736052-46-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)cyclohexyl]methyl]-N2-(4-methoxy-2-naphthalenyl)-5-nitro- (9CI) (CA INDEX NAME)



RN 736052-50-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)cyclohexyl]methyl]-5-nitro-N2-6-quinolinyl- (9CI) (CA INDEX NAME)



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L4   ANSWER 18 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  10 Jun 2004
GI
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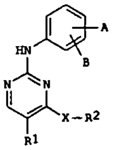

I

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AB   The title compds. [I; A, B = CN, halo, H, OH, etc.; X = O, (un)substituted
     NH; R1 = H, halo, CH2OH, alkyl, etc.; R2 = H, (un)substituted NHCO-aryl or
     alkyl] which are inhibitors of kinases useful as medications for treating
     various diseases, were prepared  E.g., a multi-step synthesis of
     5-bromo-4-[2-(1H-imidazol-4-yl)ethylamino]-2-(4-pyrrolidin-1-
     ylmethylphenylamino)pyrimidine, starting from 5-bromouracil, was given.
     Biol. data for inhibition of Akt-2, Chk-1, and VEGFR-II (KDR) were given.
     The pharmaceutical composition comprising the compds. I is claimed.
ACCESSION NUMBER:        2004:467870  HCAPLUS
DOCUMENT NUMBER:         141:38625
TITLE:                   Preparation of Chk-, pdk- and akt-inhibitory
                         pyrimidines
INVENTOR(S):             Bryant, Judi; Kochanny, Monica; Yuan, Shendong; Khim,
                         Seock-Kuy; Buckman, Brad; Arnaiz, Damian; Boemer, Ulf;
                         Briem, Hans; Esperling, Peter; Huwe, Christoph;
                         Kuhnke, Joachim; Schaefer, Martina; Wortmann, Lars;
                         Kosemund, Dirk; Eckle, Emil; Feldman, Richard;
                         Phillips, Gary
PATENT ASSIGNEE(S):      Schering Aktiengesellschaft, Germany
SOURCE:                  PCT Int. Appl., 293 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                English
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE       APPLICATION NO.          DATE
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     WO 2004048343        A1    20040610   WO 2003-EP13443          20031128
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO,
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
             TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2502970           AA    20040610   CA 2003-2502970          20031128
     AU 2003288198        A1    20040618   AU 2003-288198           20031128
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L4   ANSWER 18 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
     US 2004186118        A1    20040923   US 2003-722591           20031128
     EP 1565446           A1    20050824   EP 2003-780086           20031128
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     BR 2003016680        A     20051018   BR 2003-16680            20031128
     JP 2006508997        T2    20060316   JP 2004-554522           20031128
     NO 2005003144        A     20050627   NO 2005-3144             20050627
PRIORITY APPLN. INFO.:                     EP 2002-26607       A    20021128
                                           WO 2003-EP13443     W    20031128
OTHER SOURCE(S):         MARPAT 141:38625
IT   702673-51-6P 702673-52-7P 702673-53-8P
     702673-55-0P 702679-23-0P 702679-24-1P
     702679-25-2P 702679-26-3P 702679-27-4P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of Chk-, pdk- and akt-inhibitory pyrimidines)
RN   702673-51-6  HCAPLUS
CN   Phenol, 3-[[5-nitro-4-(2-propynylamino)-2-pyrimidinyl]amino]- (9CI)  (CA
     INDEX NAME)
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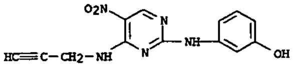

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RN   702673-52-7  HCAPLUS
CN   Benzeneacetic acid, 4-[[5-nitro-4-(2-propynylamino)-2-pyrimidinyl]amino]-,
     ethyl ester (9CI)  (CA INDEX NAME)
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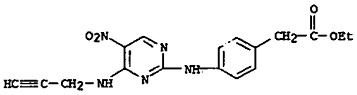

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RN   702673-53-8  HCAPLUS
CN   2,4-Pyrimidinediamine, N2-[3-(4-bromo-1-methyl-1H-pyrazol-3-yl)phenyl]-5-
     nitro-N4-2-propynyl- (9CI)  (CA INDEX NAME)
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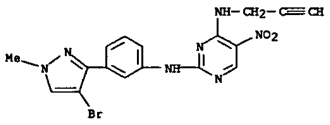

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RN   702673-55-0  HCAPLUS
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L4   ANSWER 18 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
CN   Phenol, 4-[[5-nitro-4-(2-propynylamino)-2-pyrimidinyl]amino]- (9CI)  (CA
     INDEX NAME)
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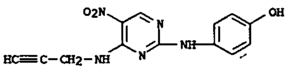

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RN   702679-23-0  HCAPLUS
CN   Benzoic acid, 2-[[5-nitro-4-(2-propynylamino)-2-pyrimidinyl]amino]-, ethyl
     ester (9CI)  (CA INDEX NAME)
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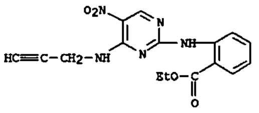

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     ester (9CI)  (CA INDEX NAME)
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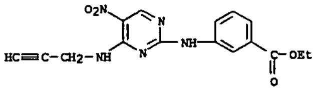

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CN   Benzoic acid, 4-[[5-nitro-4-(2-propynylamino)-2-pyrimidinyl]amino]-, ethyl
     ester (9CI)  (CA INDEX NAME)
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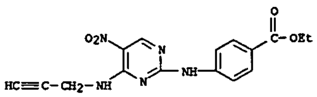

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CN   Benzeneethanol, 2-[[5-nitro-4-(2-propynylamino)-2-pyrimidinyl]amino]-
     (9CI)  (CA INDEX NAME)
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L4   ANSWER 18 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
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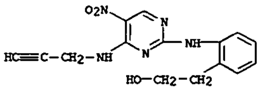

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RN   702679-27-4  HCAPLUS
CN   Benzeneethanol, 4-[[5-nitro-4-(2-propynylamino)-2-pyrimidinyl]amino]-
     (9CI)  (CA INDEX NAME)
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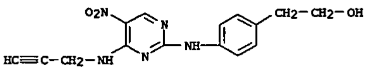

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REFERENCE COUNT:         2         THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
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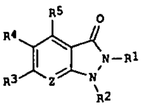
L4 ANSWER 19 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 07 May 2004
GI


I

AB The present invention provides compds. of formula (I). [Wherein R1, R2 = H or a nitrogen protecting group; one of R3 or R4 = R and the other one of R3 or R4 = -Q1-A-Q2-Y; wherein Q1 = a valence bond, NRa, C(Ra)2, S, O, SO2, NRaSO2, SO2NRa, CO, NRaCO, CONRa, OC(O), C(O)O, OC(O)NRa, 1,2-cyclopropanedilyl, 1,2-cyclobutanediyl, or 1,3-cyclobutanediyl, optionally substituted C2-4 alkylidene, etc.; wherein Ra = H, each optionally substituted C1-4 aliphatic; A = optionally substituted 5-to 7-membered monocyclic or 8- to 10-membered bicyclic aryl, heteroaryl, heterocyclic, carbocyclic ring, or C2-6 alkylidene, etc.; Q2 = NRc, SO, O, or C(Rc)2; wherein Rc = H, optionally substituted C1-4 aliphatic; Y = each optionally substituted 5- to 7-membered monocyclic or 8- to 10 membered bicyclic aryl, heteroaryl, heterocyclic, or carbocyclic ring; R5 = R; Z = N, CR6; wherein R6 = R; R = H, halo, Q-halogen, cyano, Q-CN, NO2, Q-NO2, R7, Q-R7; Q = optionally substituted C1-4 alkylidene; wherein one or more methylene units of Q is optionally replaced by O, S, NR7, NR7CO, NR7CONR7, NR7CO2, CO, CO2, CONR7, OC(O)NR7, SO2, SO2NR7, NR7SO2, NR7SO2NR7, C(O)C(O), or C(O)C(R7)2C(O); wherein R7 = H, each optionally substituted aliphatic, heteroaliph., aryl or heteroaryl]. The compds. I and pharmaceutically acceptable compns. thereof, are useful generally as protein kinase inhibitors, particularly as inhibitors of protein kinase PRAK, protein kinase GSK3, protein kinase ERK2, protein kinase CDK2, MAP kinase-activated protein kinase 2 (MK2), SRC kinase, protein kinase SYK, and protein kinase Aurora-2. Accordingly, the compds. I and compns. of the invention are useful for treating or lessening the severity of a disease or condition selected from cardiovascular disease, diabetes, neurol. disorders (e.g. Alzheimer's disease), immunodeficiency disorders, inflammatory diseases, allergic diseases, autoimmune diseases, destructive bone disorders such as osteoporosis, proliferative disorders, infectious diseases, and viral diseases. Thus, a solution of (2-chloroquinazolin-4-yl)(5-cyclopropyl-1H-pyrazol-3-yl)amine (50.0 mg, 0.175 mmol) and 6-amino-3-oxo-2,3-dihydroindazole-1-carboxylic acid tert-Bu ester (69.8 mg. 0.280 mmol) in NMP (1.0 mL) was heated up to 100° for 6 h to give, after workup, acidification with CF3CO2H, and HPLC purification, 6-[[4-[(5-cclopropyl-1H-pyrazol-3-yl)amino]quinazolin-2-yl]amino]-1,2-dihydroindazol-3-one trifluoroacetate. Some compds. of the formula I were shown to have Ki of <0.1 μM for GSK-3 and Aurora-2 and <1.0 μM for CDK-2, ERK2, PRAK, SRC, SYK, and MK2.

ACCESSION NUMBER:	2004:370926 HCAPLUS
DOCUMENT NUMBER:	140:391292
TITLE:	Preparation of indazolinone compositions useful as kinase inhibitors
INVENTOR(S):	Aronov, Alex; Lauffer, David J.; Li, Huan Qui; Tomlinson, Ronald Charles; Li, Pan
PATENT ASSIGNEE(S):	Vertex Pharmaceuticals Incorporated, USA

L4 ANSWER 19 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

SOURCE:	PCT Int. Appl., 260 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

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     PATENT NO.          KIND    DATE         APPLICATION NO.         DATE
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     WO 2004037814        A1     20040506     WO 2003-US34065         20031027
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
             UG, US, UZ, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
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     AU 2003286711        A1     20040513     AU 2003-286711          20031027
     US 2004167121        A1     20040826     US 2003-694534          20031027
PRIORITY APPLN. INFO.:                        US 2002-421398P      P  20021025
                                              WO 2003-US34065      W  20031027
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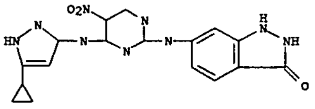
OTHER SOURCE(S): MARPAT 140:391292

IT **685867-17-8P**, 6-[[4-[(5-Cyclopropyl-1H-pyrazol-3-yl)amino]-5-nitropyrimidin-2-yl]amino]-1,2-dihydroindazol-3-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indazolinone derivs. as kinase inhibitors for treating or lessening severity of diseases or conditions)

RN 685867-17-8 HCAPLUS

CN 3H-Indazol-3-one, 6-[[4-[(5-cyclopropyl-1H-pyrazol-3-yl)amino]-5-nitro-2-pyrimidinyl]amino]-1,2-dihydro- (9CI) (CA INDEX NAME)



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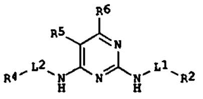
L4 ANSWER 20 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Feb 2004
GI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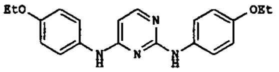
II

AB The present invention provides methods of treating or preventing autoimmune diseases with 2,4-pyrimidinediamine compds., as well as methods of treating, preventing or ameliorating symptoms associated with such diseases. Title compds. I [wherein L1 and L2 = independently a bond or a linker; R2 = (un)substituted alkyl, (hetero)cycloalkyl, or (hetero)aryl; R4 = H or R2; R5 = R6 or (un)substituted alkyl, alkenyl, or alkynyl; R6 = independently H, an electroneg. group, protected alc. or thiol, haloalkyl(oxy), halo, CN, NC, OCN, SCN, NO, NO2, N3, or (un)substituted amino, sulfamoyl(oxy), acyl, carboxy, carbamoyl, (hetero)aryl(alkyl), etc.; with provisos and exclusions; and salts, hydrates, solvates, N-oxides, and prodrugs thereof] were prepared as inhibitors of the IgE and/or IgG receptor signaling cascades that lead to the release of chemical mediators. For example, coupling of 2,4-dichloropyrimidine with 4-ethoxyaniline in EtOH provided N2,N4-bis(4-ethoxyphenyl)-2,4-pyrimidinediamine (II). The latter inhibited degranulation of bone marrow derived mast cells challenged with anti-IgE and ionomycin with IC50 values of 4.5 μM and 4.4 μM, resp. Thus, I and their pharmaceutical compns. are useful in the treatment and prevention of diseases characterized by, caused by, or associated with the release of chemical mediators via degranulation of mast, basophil, neutrophil, or eosinophil cells and other processes effected by activation of the IgE and/or IgG receptor signaling cascades. Specific examples of autoimmune diseases that can be treated or prevented with I and their pharmaceutical compns. include rheumatoid arthritis, systemic lupus erythematosis, and multiple sclerosis (no data).

ACCESSION NUMBER:	2004:142963 HCAPLUS
DOCUMENT NUMBER:	140:199334
TITLE:	Preparation of 2,4-pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of autoimmune diseases
INVENTOR(S):	Singh, Rajinder; Argade, Ankush; Payan, Donald G.; Clough, Jeffrey; Keim, Holger; Sylvain, Catherine; Li, Hui; Bhamidipati, Somasekhar
PATENT ASSIGNEE(S):	Rigel Pharmaceuticals, USA
SOURCE:	PCT Int. Appl., 811 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	2

L4 ANSWER 20 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PATENT INFORMATION:

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     CA 2492325           AA     20040219     CA 2003-2492325         20030729
     AU 2003265336        A1     20040225     AU 2003-265336          20030729
     EP 1534286           A1     20050601     EP 2003-784871          20030729
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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     US 2005038243        A1     20050217     US 2004-858343          20040601
     US 2005209230        A1     20050922     US 2004-911684          20040803
     SE 2005000203        A      20050329     SE 2005-203             20050127
     NO 2005001069        A      20050228     NO 2005-1069            20050228
     US 2006025410        A1     20060202     US 2005-149105          20050608
     US 2006035916        A1     20060216     US 2005-148746          20050608
     US 2006058292        A1     20060316     US 2005-149418          20050608
PRIORITY APPLN. INFO.:                        US 2002-399673P      P  20020729
                                              US 2003-443949P      P  20030131
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                                              US 2003-631029       A  20030729
                                              US 2002-353267P      P  20020201
                                              US 2002-353333P      P  20020201
                                              US 2002-434277P      P  20021217
                                              US 2003-355543       A1 20030131
                                              WO 2003-US24087      W  20030729
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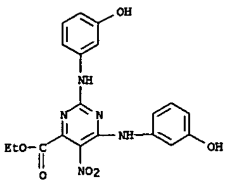
OTHER SOURCE(S): MARPAT 140:199334

IT **575475-97-7P 575475-98-8P 575482-23-4P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(IgE and/or IgG receptor modulator; preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of autoimmune diseases)

RN 575475-97-7 HCAPLUS

CN 4-Pyrimidinecarboxylic acid, 2,6-bis[(3-hydroxyphenyl)amino]-5-nitro-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 20 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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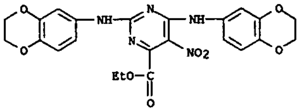

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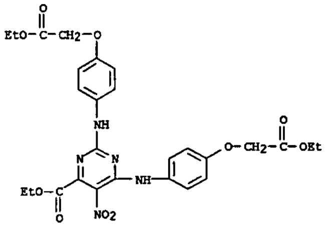
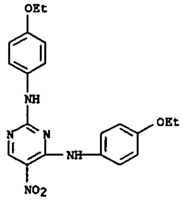
CN 4-Pyrimidinecarboxylic acid, 2,6-bis[[4-(2-ethoxy-2-oxoethoxy)phenyl]amino]-5-nitro-, ethyl ester (9CI) (CA INDEX NAME)



IT **362620-72-2P 575475-32-0P 575475-33-1P 575475-34-2P 575475-35-3P 575479-43-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(IgE and/or IgG receptor modulator; prepn. of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of autoimmune diseases)

L4 ANSWER 20 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 362620-72-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N,N'-bis(4-ethoxyphenyl)-5-nitro- (9CI) (CA INDEX NAME)



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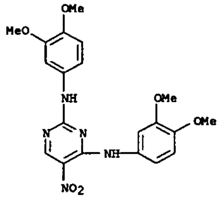
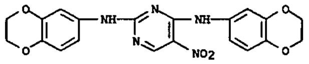
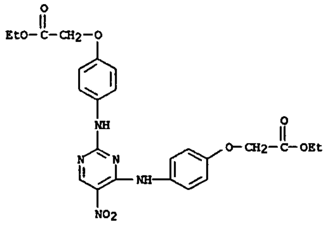


RN 575475-33-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N,N'-bis(2,3-dihydro-1,4-benzodioxin-6-yl)-5-nitro- (9CI) (CA INDEX NAME)



RN 575475-34-2 HCAPLUS
CN Acetic acid, 2,2'-[(5-nitro-2,4-pyrimidinediyl)bis(imino-4,1-phenyleneoxy)]bis-, diethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 20 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 575475-35-3 HCAPLUS
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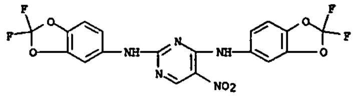
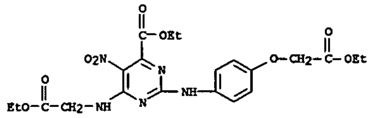
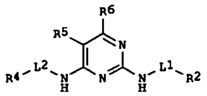


RN 575479-43-5 HCAPLUS
CN 4-Pyrimidinecarboxylic acid, 2-[[4-(2-ethoxy-2-oxoethoxy)phenyl]amino]-6-[(2-ethoxy-2-oxoethyl)amino]-5-nitro-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 21 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 08 Aug 2003
GI



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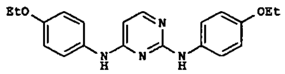

II

AB Title compds. I [wherein L1 and L2 = independently a bond or a linker; R2 = (un)substituted alkyl, (hetero)cycloalkyl, or (hetero)aryl; R4 = H or R2; R5 = R6 or (un)substituted alkyl, alkenyl, or alkynyl; R6 = independently H, an electroneg. group, protected alc. or thiol, haloalkyl(oxy), halo, CN, NC, OCN, SCN, NO, NO2, N3, or (un)substituted amino, sulfamoyl(oxy), acyl, carboxy, carbamoyl, (hetero)aryl(alkyl), etc.; with provisos and exclusions; and salts, hydrates, solvates, N-oxides, and prodrugs thereof] were prepared as inhibitors of the IgE and/or IgG receptor signaling cascades that lead to the release of chemical mediators. For example, coupling of 2,4-dichloropyrimidine with 4-ethoxyaniline in EtOH provided N2,N4-bis(4-ethoxyphenyl)-2,4-pyrimidinediamine (II). The latter inhibited degranulation of bone marrow derived mast cells challenged with anti-IgE and ionomycin with IC50 values of 4.5 μM and 4.4 μM, resp. Thus, I and their pharmaceutical compns. are useful in the treatment and prevention of diseases characterized by, caused by, or associated with the release of chemical mediators via degranulation of mast, basophil, neutrophil, or eosinophil cells and other processes effected by activation of the IgE and/or IgG receptor signaling cascades. The treatment and prevention of allergic diseases, low grade scarring, diseases associated with tissue destruction, diseases associated with tissue inflammation, inflammation, and scarring are targeted uses (no data).

ACCESSION NUMBER:	2003:610204 HCAPLUS
DOCUMENT NUMBER:	139:164801
TITLE:	Preparation of 2,4-pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction
INVENTOR(S):	Singh, Rajinder; Argade, Ankush; Payan, Donald G.; Molineaux, Susan; Holland, Sacha J.; Clough, Jeffrey; Keim, Holger; Bhamidipati, Somasekhar; Sylvain, Catherine; Li, Weigun; Rossi, Alexander B.
PATENT ASSIGNEE(S):	Rigel Pharmaceuticals, Inc., USA
SOURCE:	PCT Int. Appl., 648 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	2
PATENT INFORMATION:	

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L4   ANSWER 21 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
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             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2474277           AA    20030807   CA 2003-2474277        20030131
     US 2004029902        A1    20040212   US 2003-355543         20030131
     EP 1471915           A2    20041103   EP 2003-707654         20030131
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     JP 2005516046        T2    20050602   JP 2003-563490         20030131
     CN 1625400           A     20050608   CN 2003-803180         20030131
     BR 2003007355        A     20060411   BR 2003-7355           20030131
     US 2005038243        A1    20050217   US 2004-858343         20040601
     US 2005209230        A1    20050922   US 2004-911684         20040803
     NO 2004003632        A     20041026   NO 2004-3632           20040831
     US 2006025410        A1    20060202   US 2005-149105         20050608
     US 2006035916        A1    20060216   US 2005-148746         20050608
     US 2006058292        A1    20060316   US 2005-149418         20050608
PRIORITY APPLN. INFO.:                     US 2002-353267P     P  20020201
                                           US 2002-353333P     P  20020201
                                           US 2002-399673P     P  20020729
                                           US 2002-434277P     P  20021217
                                           US 2003-355543      A1 20030131
                                           WO 2003-US3022      W  20030131
OTHER SOURCE(S):         MARPAT 139:164801
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IT **575475-97-7P 575475-98-8P 575482-23-4P**

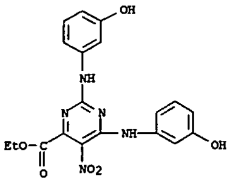
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(IgE and/or IgG receptor modulator; preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction)

RN 575475-97-7 HCAPLUS

CN 4-Pyrimidinecarboxylic acid, 2,6-bis[(3-hydroxyphenyl)amino]-5-nitro-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 575475-98-8 HCAPLUS

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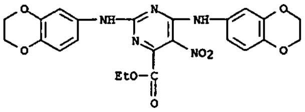

RN 575482-23-4 HCAPLUS

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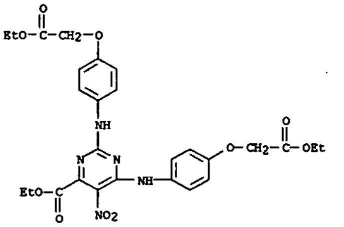


IT **362620-72-2P 575475-32-0P 575475-33-1P 575475-34-2P 575475-35-3P 575479-43-5P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

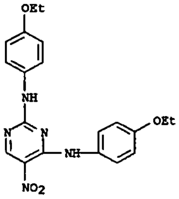
L4 ANSWER 21 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

(Uses)

(IgE and/or IgG receptor modulator; prepn. of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction)

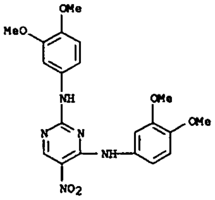
RN 362620-72-2 HCAPLUS

CN 2,4-Pyrimidinediamine, N,N'-bis(4-ethoxyphenyl)-5-nitro- (9CI) (CA INDEX NAME)



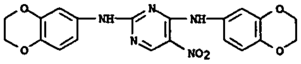
RN 575475-32-0 HCAPLUS

CN 2,4-Pyrimidinediamine, N,N'-bis(3,4-dimethoxyphenyl)-5-nitro- (9CI) (CA INDEX NAME)



RN 575475-33-1 HCAPLUS

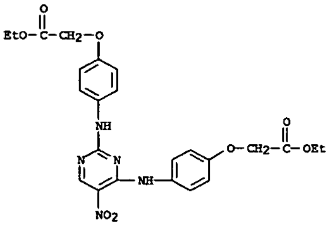
CN 2,4-Pyrimidinediamine, N,N'-bis(2,3-dihydro-1,4-benzodioxin-6-yl)-5-nitro- (9CI) (CA INDEX NAME)



RN 575475-34-2 HCAPLUS

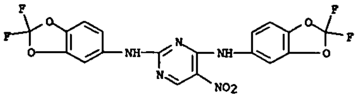
CN Acetic acid, 2,2'-[(5-nitro-2,4-pyrimidinediyl)bis(imino-4,1-phenyleneoxy)]bis-, diethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



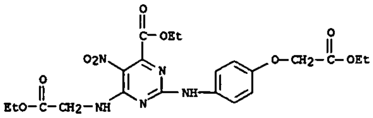
RN 575475-35-3 HCAPLUS

CN 2,4-Pyrimidinediamine, N,N'-bis(2,2-difluoro-1,3-benzodioxol-5-yl)-5-nitro- (9CI) (CA INDEX NAME)



RN 575479-43-5 HCAPLUS

CN 4-Pyrimidinecarboxylic acid, 2-[[4-(2-ethoxy-2-oxoethoxy)phenyl]amino]-6-[(2-ethoxy-2-oxoethyl)amino]-5-nitro-, ethyl ester (9CI) (CA INDEX NAME)



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L4   ANSWER 22 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  09 May 2003
GI
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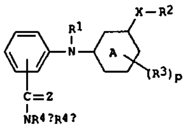

I

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AB   Aminobenzamide derivs. (I), N-oxides, pharmaceutically acceptable addition
     salts, quaternary amines, and stereochem. isomeric forms thereof [wherein
     ring A = pyridyl, pyrimidinyl, pyrazinyl, pyridazinyl; R1 = H, aryl, CHO,
     C1-6 alkylcarbonyl, optionally substituted C1-6 alkyl, C1-6
     alkyloxycarbonyl, optionally substituted C1-6 alkyloxy-C1-6 alkylcarbonyl;
     X = a direct bond or a linker atom or group; Z = O, S; R2 = H, each
     (un)substituted C1-10 alkyl, C2-10 alkenyl, C2-10 alkynyl, or carbocycle
     or heterocycle group; R3 = H, HO, halo, each optionally substituted C1-6
     alkyl, C2-6 alkenyl, or C2-6 alkynyl, C1-6 alkyloxy, C1-6 alkylthio; C1-6
     alkyloxycarbonyl, C1-6 alkylcarbonyloxy, carboxyl, cyano, nitro, amino,
     mono- or di(C1-6 alkyl)amino, polyhalo-C1-6 alkyl, polyhalo-C1-6 alkyloxy,
     polyhalo-C1-6 alkylthio, R21, R21-C1-6 alkyl, R21O, R21S, R21CO, R21S(O)n,
     NHCHO, CONHNH2, etc.; R4a, R4b = H, R8, Y1-NR9-Y2-NR10R11, Y1-NR9-Y1-R8,
     Y1-NR9R10; wherein n = 1,2; R21 = (un)substituted monocyclic, bicyclic or
     tricyclic (partially) saturated carbocycle or heterocycle, monocyclic,
     bicyclic or tricyclic aromatic carbocycle or heterocycle; Y1, Y2 = a direct
     bond, a linker group; R8 = C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, etc.;
     R9, R10, R11 = H, R8, etc.; p = 1-3] are prepared  These compds. are useful
     for the prevention or the treatment of diseases mediated through GSK3
     including bipolar disorder (in particular manic depression), diabetes,
     Alzheimer's disease, leukopenia, FTDP-17 (fronto-temporal dementia associated
     with Parkinson's disease), cortico-basal degeneration, progressive
     supranuclear palsy, multiple system atrophy, Pick's disease, Niemann
     Pick's disease type C, Dementia Pugilistica, dementia with tangles only,
     dementia with tangles and calcification, Down syndrome, myotonic
     dystrophy, Parkinsonism-dementia complex of Guam, AIDS related dementia,
     Postencephalic Parkinsonism, prion diseases with tangles, subacute
     sclerosing panencephalitis, frontal lobe degeneration (FLD), argyrophilic
     grains disease, subacute sclerotizing panencephalitis (SSPE) (late
     complication of viral infections in the central nervous system),
     inflammatory diseases, cancer, dermatol. disorders, neuronal damage,
     schizophrenia, and pain.  Thus, a solution of 2-chloro-5-nitro-N-
     (phenylmethyl)-4-pyrimidinamine (0.012 mol), 3-aminobenzamide (0.012 mol)
     and Et3N (0.012 mol) in DMF (50 mL) was stirred for 2 h at 60° to
     give 77% 3-[[4-benzylamino-5-nitropyrimidin-2-yl]amino]benzamide (II).  II
     and 3-[(4-benzyloxypyrimidin-2-yl)amino]benzamide showed pIC50(M) of 6.74
     and 5.85, resp., against GSK3β.
ACCESSION NUMBER:         2003:356429  HCAPLUS
DOCUMENT NUMBER:          138:368902
TITLE:                    Preparation of aminobenzamide derivatives as glycogen
                          synthase kinase 3β inhibitors
INVENTOR(S):              Freyne, Eddy Jean Edgard; Buijnsters, Peter Jacobus
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L4   ANSWER 22 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
                          Johannes Antonius; Willems, Marc; Embrechts, Werner
                          Constant Johan; Janssen, Paul Adriaan Jan; Lewi,
                          Paulus Joannes; Heeres, Jan; De Jonge, Marc Rene;
                          Koymans, Lucien Maria Henricus; Daeyaert, Frederik
                          Frans Desire; Kukla, Michael Joseph; Geerts, Hugo
                          Alfons Gabriel; Nuydens, Rony Maria; Mercken, Marc
                          Hubert; Ludovici, Donald William
PATENT ASSIGNEE(S):       Janssen Pharmaceutica N.V., Belg.
SOURCE:                   PCT Int. Appl., 87 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

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     WO 2003037877        A1     20030508      WO 2002-EP12079          20021029
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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
             CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2463823           AA     20030508      CA 2002-2463823          20021029
     EP 1442024           A1     20040804      EP 2002-802307           20021029
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
     BR 2002013790        A      20041207      BR 2002-13790            20021029
     JP 2005507420        T2     20050317      JP 2003-540159           20021029
     NO 2004002253        A      20040601      NO 2004-2253             20040601
     US 2006063789        A1     20060323      US 2005-493446           20050309
PRIORITY APPLN. INFO.:                         EP 2001-204192       A   20011101
                                               WO 2002-EP12079      W   20021029
OTHER SOURCE(S):          MARPAT 138:368902
IT   521304-18-7P
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (preparation of aminobenzamide derivs. as glycogen synthase kinase 3β
        (GSK3β) inhibitors for preventing or treating GSK3β-mediated
        diseases)
RN   521304-18-7  HCAPLUS
CN   Benzamide, 3-[[2-[[3-(1-methyl-1H-imidazol-2-yl)phenyl]amino]-5-nitro-4-
     pyrimidinyl]amino]-  (9CI)  (CA INDEX NAME)
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L4   ANSWER 22 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
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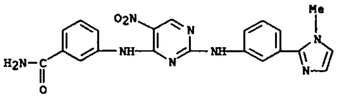

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IT   521304-07-4P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of aminobenzamide derivs. as glycogen synthase kinase 3β
        (GSK3β) inhibitors for preventing or treating GSK3β-mediated
        diseases)
RN   521304-07-4  HCAPLUS
CN   Benzamide, 3-[[5-nitro-4-[(phenylmethyl)amino]-2-pyrimidinyl]amino]-  (9CI)
       (CA INDEX NAME)
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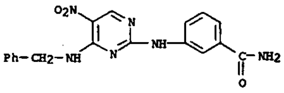

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REFERENCE COUNT:          11     THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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ED   Entered STN:  25 Apr 2003
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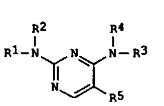

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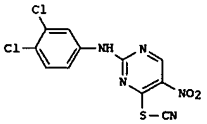

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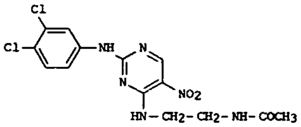

III

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AB   Title compds. I [R1 = H, alkyl; R2 = (un)substituted alkyl; R3 = H, alkyl;
     R4 = (un)substituted alkyl; R5 = halo] and their pharmaceutically
     acceptable salts were prepared  For example, condensation of
     thiocyanatopyrimide II, e.g., prepared from 3,4-dichloroaniline and
     2-chloro-4-thiocyanato-5-nitropyrimidine in one step, and
     acetylaminoethylamine provided trisubstituted pyrimidine III in 88% yield.
     In CDK1/CyclinB1 kinase inhibition studies, 88-examples of compds. I
     exhibited IC50 values more than 100 nM.  Compds. I are claimed useful for
     the treatment of diseases characterized by abnormal cell proliferation.
ACCESSION NUMBER:         2003:319721  HCAPLUS
DOCUMENT NUMBER:          138:321292
TITLE:                    Preparation of 2,4,5-trisubstituted pyrimidines as
                          cyclin dependent kinase inhibitors
INVENTOR(S):              Dahmann, Georg; Himmelsbach, Frank; Wittneben, Helmut;
                          Pautsch, Alexander; Prokopowicz, Anthony S.; Krist,
                          Bernd; Schnapp, Gisela; Steegmaier, Martin; Lenter,
                          Martin; Schoop, Andreas; Steurer, Steffen; Spevak,
                          Walter
PATENT ASSIGNEE(S):       Boehringer Ingelheim Pharma K.-G., Germany; Boehringer
                          Ingelheim Pharmaceuticals, Inc.; Boehringer Ingelheim
                          International G.m.b.H.
SOURCE:                   PCT Int. Appl., 278 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 German
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND    DATE          APPLICATION NO.          DATE
     ---------------     ----    --------      --------------------     --------
     WO 2003032997        A1     20030424      WO 2002-EP11453          20021014
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
L4   ANSWER 23 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
             CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2463989          AA      20030424    CA 2002-2463989          20021014
     EP 1438053          A1      20040721    EP 2002-774710           20021014
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
     JP 2005509624       T2      20050414    JP 2003-535800           20021014
     US 2003171359       A1      20030911    US 2002-271763           20021016
PRIORITY APPLN. INFO.:                       US 2001-330145P     P    20011017
                                             WO 2002-EP11453     W    20021014
OTHER SOURCE(S):         MARPAT 138:321292
IT   514832-07-6P, 2-(4-Chlorophenylamino)-4-(2-aminoethylamino)-5-
     nitropyrimidine 514834-99-2P, 2-(4-Chlorophenylamino)-4-((3-
     (ethoxycarbonyl)propyl)amino)-5-nitropyrimidine 514836-83-0P,
     2-(4-Chlorophenylamino)-4-(((ethoxycarbonyl)methyl)amino)-5-
     nitropyrimidine 514836-84-1P, 2-(4-Chlorophenylamino)-4-[(2-
     (ethoxycarbonyl)ethyl)amino]-5-nitropyrimidine 514836-96-5P,
     2-(3,4-Dichlorophenylamino)-4-[(2-ethoxycarbonylethyl)amino]-5-
     nitropyrimidine
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (drug candidate; preparation of trisubstituted pyrimidines as cyclin
        dependent kinase inhibitors)
RN   514832-07-6  HCAPLUS
CN   2,4-Pyrimidinediamine, N4-(2-aminoethyl)-N2-(4-chlorophenyl)-5-nitro-
     (9CI)  (CA INDEX NAME)
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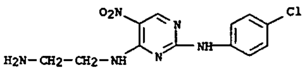

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RN   514834-99-2  HCAPLUS
CN   Butanoic acid, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-
     , ethyl ester (9CI)  (CA INDEX NAME)
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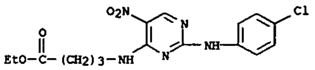

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RN   514836-83-0  HCAPLUS
CN   Glycine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]-, ethyl ester
     (9CI)  (CA INDEX NAME)
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L4   ANSWER 23 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
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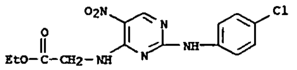

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RN   514836-84-1  HCAPLUS
CN   β-Alanine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]-,
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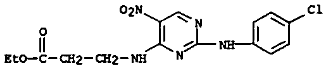

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RN   514836-96-5  HCAPLUS
CN   β-Alanine, N-[2-[(3,4-dichlorophenyl)amino]-5-nitro-4-pyrimidinyl]-,
     ethyl ester (9CI)  (CA INDEX NAME)
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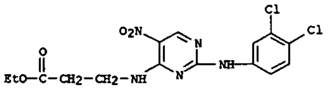

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IT   514830-60-5P, 2-(3,4-Dichlorophenylamino)-4-(((4-
     aminomethylcyclohexyl)methyl)amino)-5-nitropyrimidine 514830-66-1P
     , 2-(4-Amino-3,5-dichlorophenylamino)-4-[bis-(2-hydroxyethyl)amino]-5-
     nitropyrimidine 514830-67-2P, 2-(4-Aminosulfonylphenylamino)-4-
     [3-(2-oxopyrrolidin-1-yl)propylamino]-5-nitropyrimidine
     514830-72-9P, 2-(4-Carboxyphenylamino)-4-[N-(3-
     (dimethylamino)propyl)-N-methylamino]-5-nitropyrimidine
     514830-77-4P, 2-(4-Carboxyphenylamino)-4-((trans-4-
     (dimethylamino)cyclohexyl)amino)-5-nitropyrimidine 514830-93-4P,
     2-(4-Chlorophenylamino)-4-(3-aminocyclohexylamino)-5-nitropyrimidine
     514831-03-9P, 2-(4-Chlorophenylamino)-4-[N-(1-methylpiperidin-4-
     yl)-N-methylamino]-5-nitropyrimidine 514831-07-3P,
     2-(4-Chlorophenylamino)-4-[(1S)-1-carboxyethylamino]-5-nitropyrimidine
     514831-18-6P, 2-(4-Chlorophenylamino)-4-[(2-(3-hydroxyphenyl)-2-
     hydroxyethyl)amino]-5-nitropyrimidine 514831-34-6P
     514831-35-7P, 2-(4-Aminosulfonylphenylamino)-4-(((4-
     aminomethylcyclohexyl)methyl)amino)-5-nitropyrimidine 514831-42-6P
     , 2-(4-Chlorophenylamino)-4-[N-methyl-N-(2-cyanoethyl)amino]-5-
     nitropyrimidine 514831-46-0P, 2-(4-Chlorophenylamino)-4-(4-
     carboxybutylamino)-5-nitropyrimidine 514831-52-8P,
     2-(3-Nitrophenylamino)-4-(((4-aminomethylcyclohexyl)methyl)amino)-5-
     nitropyrimidine 514831-54-0P, 2-(4-Methoxycarbonylphenylamino)-4-
     (((4-aminomethylcyclohexyl)methyl)amino)-5-nitropyrimidine
     514831-55-1P, 2-(4-Chlorophenylamino)-4-[3-(2-oxopyrrolidin-1-
     yl)propylamino]-5-nitropyrimidine 514831-58-4P,
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L4   ANSWER 23 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
     2-(4-Benzylaminocarbonylphenylamino)-4-(((4-aminomethylcyclohexyl)methyl)a
     mino)-5-nitropyrimidine 514831-60-8P, 2-(4-Amino-3,5-
     dichlorophenylamino)-4-(((4-aminomethylcyclohexyl)methyl)amino)-5-
     nitropyrimidine 514831-66-4P, 2-(4-Chlorophenylamino)-4-(5-
     aminopentylamino)-5-nitropyrimidine 514831-70-0P,
     2-(4-Chlorophenylamino)-4-(2-methoxyethylamino)-5-nitropyrimidine
     514831-75-5P, 2-(4-Chloro-3-methylphenylamino)-4-(((4-
     aminomethylcyclohexyl)methyl)amino)-5-nitropyrimidine 514831-82-4P
     , 2-(4-Chlorophenylamino)-4-[N-(2-hydroxybenzyl)-N-methylamino]-5-
     nitropyrimidine 514831-83-5P, 2-((4-
     Phenylaminocarbonylphenyl)amino)-4-(((4-aminomethylcyclohexyl)methyl)amino
     )-5-nitropyrimidine 514832-09-8P, 2-(4-Chlorophenylamino)-4-[(2-
     (acetylamino)ethyl)amino]-5-nitropyrimidine 514832-11-2P,
     2-(4-Chlorophenylamino)-4-[4-(dimethylamino)butylamino]-5-nitropyrimidine
     514832-14-5P, 2-(4-Carboxyphenylamino)-4-[N-(2-hydroxyethyl)-N-
     (benzyl)amino]-5-nitropyrimidine 514832-18-9P,
     2-(4-Chlorophenylamino)-4-((trans-4-carboxycyclohexyl)amino)-5-
     nitropyrimidine 514832-20-3P, 2-(4-Carboxyphenylamino)-4-[3-(2-
     oxopyrrolidin-1-yl)propylamino]-5-nitropyrimidine 514832-21-4P,
     2-(4-Chlorophenylamino)-4-((2-morpholinoethyl)amino)-5-nitropyrimidine
     514832-23-6P, 2-[(4-Chlorophenyl)amino]-4-[(2-(1H-imidazol-4-
     yl)ethyl)amino]-5-nitropyrimidine 514832-24-7P,
     2-(4-Chlorophenylamino)-4-[(2-(4-hydroxyphenyl)-2-hydroxyethyl)amino]-5-
     nitropyrimidine 514832-25-8P, 2-(4-Chlorophenylamino)-4-[(2-(4-
     hydroxy-3-methoxyphenyl)-2-hydroxyethyl)amino]-5-nitropyrimidine
     514832-26-9P, 2-(4-Chlorophenylamino)-4-[(2-(1-methyl-2-
     pyrrolidinyl)ethyl)amino]-5-nitropyrimidine 514832-27-0P,
     2-(4-Chlorophenylamino)-4-(4-hydroxybutylamino)-5-nitropyrimidine
     514832-28-1P, 2-(4-Chlorophenylamino)-4-(6-hydroxyhexylamino)-5-
     nitropyrimidine 514832-29-2P, 2-(4-Chlorophenylamino)-4-(5-
     hydroxypentylamino)-5-nitropyrimidine 514832-30-5P,
     2-(4-Chlorophenylamino)-4-(1,1-dimethyl-2-hydroxyethylamino)-5-
     nitropyrimidine 514832-31-6P, 2-(4-Carboxyphenylamino)-4-[(2-(3-
     hydroxyphenyl)ethyl)amino]-5-nitropyrimidine 514832-34-9P,
     2-(4-Carboxyphenylamino)-4-[(2-(4-hydroxyphenyl)ethyl)amino]-5-
     nitropyrimidine 514832-36-1P, 2-(3-Carboxyphenylamino)-4-[(2-(4-
     hydroxyphenyl)ethyl)amino]-5-nitropyrimidine 514832-37-2P,
     2-(3-Carboxyphenylamino)-4-[(2-(3-hydroxyphenyl)ethyl)amino]-5-
     nitropyrimidine 514832-38-3P, 2-(4-Chlorophenylamino)-4-[(2-(2-
     oxoimidazolidinyl-1-yl)ethyl)amino]-5-nitropyrimidine 514832-40-7P
     , 2-(3-Bromophenylamino)-4-(((4-aminomethylcyclohexyl)methyl)amino)-5-
     nitropyrimidine 514832-41-8P, 2-(4-Bromophenylamino)-4-(((4-
     aminomethylcyclohexyl)methyl)amino)-5-nitropyrimidine 514832-42-9P
     , 2-(4-Chlorophenylamino)-4-(1-methyl-4-piperidinylamino)-5-
     nitropyrimidine 514832-43-0P, 2-(4-Chlorophenylamino)-4-(6-
     aminohexylamino)-5-nitropyrimidine 514832-44-1P,
     2-(4-Chlorophenylamino)-4-(((3-aminomethylcyclohexyl)methyl)amino)-5-
     nitropyrimidine 514832-46-3P, 2-(3-Carboxyphenylamino)-4-(4-
     aminosulfonylbenzylamino)-5-nitropyrimidine 514832-47-4P,
     2-(4-Chlorophenylamino)-4-[N-(1-methyl-4-piperidinylmethyl)-N-methylamino]-
     5-nitropyrimidine 514832-48-5P, 2-(3-Carboxyphenylamino)-4-(((4-
     aminomethylcyclohexyl)methyl)amino)-5-nitropyrimidine 514832-49-6P
     , 2-(3-Ethoxycarbonylphenylamino)-4-(((4-aminomethylcyclohexyl)methyl)amin
     o)-5-nitropyrimidine 514832-53-2P, 2-(4-Carboxyphenylamino)-4-(4-
     hydroxybenzylamino)-5-nitropyrimidine 514832-59-8P,
     2-(4-Chlorophenylamino)-4-(trans-4-hydroxycyclohexylamino)-5-
     nitropyrimidine 514832-60-1P, 2-(4-Chlorophenylamino)-4-(4-
     aminocyclohexylamino)-5-nitropyrimidine 514832-61-2P,
     2-(4-Chlorophenylamino)-4-(4-dimethylaminocyclohexylamino)-5-
     nitropyrimidine 514832-62-3P, 2-(4-Chlorophenylamino)-4-[(1R)-1-
     carboxyethylamino]-5-nitropyrimidine 514832-63-4P,
     2-(4-Chlorophenylamino)-4-(3-aminopropylamino)-5-nitropyrimidine
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L4   ANSWER 23 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
     514832-64-5P, 2-(4-Chlorophenylamino)-4-[(3-
     (isopropylamino)propyl)amino]-5-nitropyrimidine 514832-65-6P,
     2-(4-Chlorophenylamino)-4-[((3-hydroxy-8-methyl-8-azabicyclo[3.2.1]oct-3-
     yl)methyl)amino]-5-nitropyrimidine 514832-66-7P,
     2-(4-Chlorophenylamino)-4-[(2-(3-carboxy-2-methoxyphenyl)ethyl)amino]-5-
     nitropyrimidine 514832-68-9P, 2-(4-Chlorophenylamino)-4-[bis-(2-
     hydroxyethyl)amino]-5-nitropyrimidine 514832-69-0P,
     2-(4-Chlorophenylamino)-4-(4-nitrobenzylamino)-5-nitropyrimidine
     514832-70-3P 514832-71-4P, 2-(4-Chlorophenylamino)-4-(1-
     carboxy-2,2-diphenylethylamino)-5-nitropyrimidine 514832-72-5P,
     2-(4-Chlorophenylamino)-4-(3-carboxycyclohexylamino)-5-nitropyrimidine
     514832-73-6P, 2-(4-Chlorophenylamino)-4-[(4-(2-
     carboxyethyl)cyclohexyl)amino]-5-nitropyrimidine 514832-74-7P,
     2-(4-Chlorophenylamino)-4-[(2-(3-hydroxyphenyl)ethyl)amino]-5-
     nitropyrimidine 514832-75-8P, 2-(4-Chlorophenylamino)-4-[(2-(1H-
     pyrazol-4-yl)ethyl)amino]-5-nitropyrimidine 514832-76-9P,
     2-(4-Chlorophenylamino)-4-((1-methylpiperidin-4-ylmethyl)amino)-5-
     nitropyrimidine 514832-77-0P, 2-(4-Chlorophenylamino)-4-(cis-4-
     hydroxycyclohexylamino)-5-nitropyrimidine 514832-78-1P,
     2-(4-Chlorophenylamino)-4-(((4-(N,N-dimethylaminomethyl)cyclohexyl)methyl)
     amino)-5-nitropyrimidine 514832-79-2P, 2-(4-Chlorophenylamino)-4-
     [(2-(imidazol-1-yl)ethyl)amino]-5-nitropyrimidine 514834-74-3P,
     2-(4-Chlorophenylamino)-4-[2-(dimethylamino)ethylamino]-5-nitropyrimidine
     514834-75-4P, 2-(4-Chlorophenylamino)-4-[3-(4-
     morpholinyl)propylamino]-5-nitropyrimidine 514834-76-5P,
     2-(4-Chlorophenylamino)-4-(2-carboxyethylamino)-5-nitropyrimidine
     514834-77-6P, 2-(4-Chlorophenylamino)-4-[(3-(1H-imidazol-1-
     yl)propyl)amino]-5-nitropyrimidine 514834-78-7P,
     2-(4-Chlorophenylamino)-4-((3-dimethylaminopropyl)amino)-5-nitropyrimidine
     514834-79-8P, 2-(4-Chlorophenylamino)-4-((2-
     diisopropylaminoethyl)amino)-5-nitropyrimidine 514834-80-1P,
     2-(4-Chlorophenylamino)-4-[bis-(2-methoxyethyl)amino]-5-nitropyrimidine
     514834-81-2P, 2-(4-Chlorophenylamino)-4-[N-methyl-N-(2-
     methylaminoethyl)amino]-5-nitropyrimidine 514834-82-3P,
     2-(4-Chlorophenylamino)-4-[(2-(4-pyridyl)ethyl)amino]-5-nitropyrimidine
     514834-83-4P, 2-(4-Chlorophenylamino)-4-(4-
     aminosulfonylbenzylamino)-5-nitropyrimidine 514834-84-5P,
     2-(4-Chlorophenylamino)-4-(4-pyridylmethylamino)-5-nitropyrimidine
     514834-85-6P, 2-(4-Chlorophenylamino)-4-[((3-chloro-5-
     trifluoromethyl-2-pyridyl)methyl)amino]-5-nitropyrimidine
     514834-86-7P, 2-(4-Chlorophenylamino)-4-(3-nitrobenzylamino)-5-
     nitropyrimidine 514834-88-9P, 2-(4-Chlorophenylamino)-4-[3-(1-
     pyrrolidinyl)propylamino]-5-nitropyrimidine 514834-89-0P
     514834-90-3P, 2-(4-Chlorophenylamino)-4-[((1-
     hydroxycyclohexyl)methyl)amino]-5-nitropyrimidine 514834-91-4P,
     2-(4-Chlorophenylamino)-4-[(2-(1H-indol-3-yl)ethyl)amino]-5-
     nitropyrimidine 514834-92-5P, 2-(4-Chlorophenylamino)-4-[(2-(4-
     nitro-2-pyridylamino)ethyl)amino]-5-nitropyrimidine 514834-93-6P
     , 2-(4-Chlorophenylamino)-4-((2-hydroxy-2-phenylethyl)amino)-5-
     nitropyrimidine 514834-94-7P, 2-(4-Chlorophenylamino)-4-((2-
     phenylaminoethyl)amino)-5-nitropyrimidine 514834-95-8P,
     2-(4-Chlorophenylamino)-4-[(2-(4-hydroxyphenyl)ethyl)amino]-5-
     nitropyrimidine 514834-96-9P, 2-(4-Chlorophenylamino)-4-[(2-(4-
     aminosulfonylphenyl)ethyl)amino]-5-nitropyrimidine 514834-97-0P,
     2-(4-Chlorophenylamino)-4-[(2-(1-naphthylamino)ethyl)amino]-5-
     nitropyrimidine 514834-98-1P, 2-(4-Chlorophenylamino)-4-[(2-(4-
     nitrophenyl)ethyl)amino]-5-nitropyrimidine 514835-00-8P,
     2-(4-Chlorophenylamino)-4-(((aminocarbonyl)methyl)amino)-5-nitropyrimidine
     514835-04-2P, 2-(4-Chlorophenylamino)-4-((2-tert-
     butoxycarbonylaminoethyl)amino)-5-nitropyrimidine 514835-05-3P,
     2-(4-Chlorophenylamino)-4-(((1-ethyl-2-pyrrolidinyl)methyl)amino)-5-
     nitropyrimidine 514835-07-5P, 2-(4-Chlorophenylamino)-4-[(2-(1-
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pyrrolidinyl)ethyl)amino]-5-nitropyrimidine **514835-08-6P**,
2-(4-Chlorophenylamino)-4-[(2-(1-piperidinyl)ethyl)amino]-5-
nitropyrimidine **514835-09-7P**, 2-(4-Chlorophenylamino)-4-(2-
hydroxypropylamino)-5-nitropyrimidine **514835-10-0P**,
2-(4-Chlorophenylamino)-4-(2,3-dihydroxypropylamino)-5-nitropyrimidine
514835-11-1P, 2-(4-Chlorophenylamino)-4-((2-
diethylaminoethyl)amino)-5-nitropyrimidine **514835-12-2P**,
2-(4-Chlorophenylamino)-4-[(2-(2-hydroxyethoxy)ethyl)amino]-5-
nitropyrimidine **514835-13-3P**, 2-(4-Chlorophenylamino)-4-(2-
hydroxyethylamino)-5-nitropyrimidine **514835-14-4P**,
2-(4-Chlorophenylamino)-4-(3-diethylaminopropylamino)-5-nitropyrimidine
514835-15-5P, 2-(4-Chlorophenylamino)-4-(3-hydroxypropylamino)-5-
nitropyrimidine **514835-16-6P**, 2-(4-Chlorophenylamino)-4-[(2-(1-
methyl-1H-pyrrol-2-yl)ethyl)amino]-5-nitropyrimidine **514835-17-7P**
, 2-(4-Chlorophenylamino)-4-(4-hydroxy-3-methoxybenzylamino)-5-
nitropyrimidine **514835-18-8P**, 2-(4-Chlorophenylamino)-4-((2-
methylsulfanylethyl)amino)-5-nitropyrimidine **514835-19-9P**,
2-(4-Chlorophenylamino)-4-(3-methoxypropylamino)-5-nitropyrimidine
514835-21-3P, 2-(4-Chlorophenylamino)-4-((2,2-dimethyl-3-
dimethylaminopropyl)amino)-5-nitropyrimidine **514835-22-4P**,
2-(4-Chlorophenylamino)-4-((2,2-dimethyl-3-hydroxypropyl)amino)-5-
nitropyrimidine **514835-23-5P**, 2-(4-Chlorophenylamino)-4-
cyanomethylamino-5-nitropyrimidine **514835-35-9P**,
2-(4-Chlorophenylamino)-4-[(3-[4-(3-aminopropyl)-1-
piperazinyl]propyl)amino]-5-nitropyrimidine **514835-37-1P**,
2-(4-Chlorophenylamino)-4-(cis-4-carboxycyclohexylamino)-5-nitropyrimidine
514835-39-3P, 2-(4-Chlorophenylamino)-4-((3-
dibenzylaminopropyl)amino)-5-nitropyrimidine **514835-41-7P**,
2-(4-Chlorophenylamino)-4-[(2-phenyl-1-((4-phenylbutyl)aminocarbonyl)ethyl
)amino]-5-nitropyrimidine **514835-43-9P**, 2-(4-Chlorophenylamino)-
4-[(1-aminocarbonyl-2-(4-methoxyphenyl)ethyl)amino]-5-nitropyrimidine
514835-45-1P, 2-(4-Chlorophenylamino)-4-[N-ethyl-N-(4-
pyridylmethyl)amino]-5-nitropyrimidine **514835-55-3P**,
2-(4-Chlorophenylamino)-4-(1-benzyl-3-pyrrolidinylamino)-5-nitropyrimidine
514835-56-4P 514835-57-5P, 2-(4-Chlorophenylamino)-4-[(3-
(1-piperidinyl)propyl)amino]-5-nitropyrimidine **514835-58-6P**,
2-(4-Chlorophenylamino)-4-(1-benzyl-4-piperidinylamino)-5-nitropyrimidine
514835-59-7P, 2-(4-Chlorophenylamino)-4-(4-aminomethylbenzylamino)-
5-nitropyrimidine **514835-60-0P**, 2-(4-Chlorophenylamino)-4-(4-
aminobutylamino)-5-nitropyrimidine **514835-61-1P**,
2-(4-Chlorophenylamino)-4-((3-amino-2,2-dimethylpropyl)amino)-5-
nitropyrimidine **514835-62-2P**, 2-(4-Chlorophenylamino)-4-(trans-2-
aminocyclohexylamino)-5-nitropyrimidine **514835-63-3P**,
2-(4-Chlorophenylamino)-4-[(2-{2-(2-aminoethoxy)ethoxy]ethyl)amino]-5-
nitropyrimidine **514835-64-4P**, 2-(4-Chlorophenylamino)-4-(3-
aminobenzylamino)-5-nitropyrimidine **514835-65-5P**,
2-(4-Chlorophenylamino)-4-[(2-((2-aminoethyl)sulfanyl)ethyl)amino]-5-
nitropyrimidine **514835-66-6P**, 2-(4-Chlorophenylamino)-4-[N-(2-
dimethylaminoethyl)-N-ethylamino]-5-nitropyrimidine **514835-67-7P**
, 2-(4-Chlorophenylamino)-4-[N-(3-dimethylaminopropyl)-N-methylamino]-5-
nitropyrimidine **514835-68-8P**, 2-(4-Chlorophenylamino)-4-[(3-(4-
methyl-1-piperazinyl)propyl)amino]-5-nitropyrimidine **514835-69-9P**
, 2-(4-Chlorophenylamino)-4-[N-(2-cyanoethyl)-N-(3-pyridylmethyl)amino]-5-
nitropyrimidine **514835-72-4P**, 2-(4-Chlorophenylamino)-4-[N-
benzyl-N-(2-cyanoethyl)amino]-5-nitropyrimidine **514835-73-5P**,
2-(4-Chlorophenylamino)-4-[N-benzyl-N-(2-hydroxyethyl)amino]-5-
nitropyrimidine **514835-74-6P**, 2-(4-Chlorophenylamino)-4-(3-
carboxypropylamino)-5-nitropyrimidine **514835-75-7P**,

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2-(4-Chlorophenylamino)-4-{N-benzyl-N-((ethoxycarbonyl)methyl)amino]-5-
nitropyrimidine **514835-76-8P**, 2-(4-Chlorophenylamino)-4-[N-(4-
nitrobenzyl)-N-propylamino]-5-nitropyrimidine **514835-78-0P**,
2-(4-Chlorophenylamino)-4-((cyanophenylmethyl)amino)-5-nitropyrimidine
514835-79-1P, 2-(4-Chlorophenylamino)-4-[N-benzyl-N-(4-
hydroxybutyl)amino]-5-nitropyrimidine **514835-80-4P**,
2-(4-Chlorophenylamino)-4-{N-benzyl-N-(2-hydroxymethylcyclohexyl)amino]-5-
nitropyrimidine **514835-81-5P 514835-82-6P**,
2-(4-Chlorophenylamino)-4-(5-carboxypentylamino)-5-nitropyrimidine
514835-83-7P 514835-84-8P 514835-85-9P
514835-86-0P, 2-(4-Chlorophenylamino)-4-[((1R)-1-carboxy-2-
hydroxyethyl)amino]-5-nitropyrimidine **514835-88-2P**,
2-(4-Chlorophenylamino)-4-(cis-2-aminocyclohexylamino)-5-nitropyrimidine
514835-92-8P, 2-(4-Chlorophenylamino)-4-[(3-[2-(3-
aminopropoxy)ethoxy]propyl)amino]-5-nitropyrimidine **514835-93-9P**
, 2-(4-Chlorophenylamino)-4-[N-benzyl-N-(2-hydroxy-1-phenylethyl)amino]-5-
nitropyrimidine **514835-95-1P**, 2-(4-Chlorophenylamino)-4-[(2-[2-
(2-hydroxyethoxy)ethoxy]ethyl)amino]-5-nitropyrimidine
514835-96-2P, 2-(4-Chlorophenylamino)-4-[(2-(3-
methoxycarbonylphenyl)ethyl)amino]-5-nitropyrimidine **514835-97-3P**
, 2-(4-Chlorophenylamino)-4-[(2-hydroxy-3-(4-morpholinyl)propyl)amino]-5-
nitropyrimidine **514835-98-4P**, 2-(4-Chlorophenylamino)-4-[N-
methyl-N-{6-[N-methyl-N-(2-phenylethyl)amino]hexyl}amino]-5-
nitropyrimidine **514835-99-5P**, 2-(4-Chlorophenylamino)-4-[(2-[2-
(2-aminoethyl)phenyl]ethyl)amino]-5-nitropyrimidine **514836-00-1P**
, 2-(4-Chlorophenylamino)-4-[N-(2-diethylaminoethyl)-N-ethylamino]-5-
nitropyrimidine **514836-03-4P**, 2-(4-Chlorophenylamino)-4-(N-
cyanomethyl-N-butylamino)-5-nitropyrimidine **514836-04-5P**,
2-(4-Chlorophenylamino)-4-{N-(2-dimethylaminoethyl)-N-methylamino]-5-
nitropyrimidine **514836-11-4P**, 2-(4-Chlorophenylamino)-4-[(2-[2-
(2-dimethylaminoethyl)-1-piperidinyl]ethyl)amino]-5-nitropyrimidine
514836-12-5P, 2-(4-Chlorophenylamino)-4-[(3-(2-
(diethylamino)methyl-1-piperidinyl)propyl)amino]-5-nitropyrimidine
514836-14-7P, 2-(4-Chlorophenylamino)-4-[(1-carboxy-2-(4-
chlorophenyl)ethyl)amino]-5-nitropyrimidine **514836-15-8P**,
2-(4-Chlorophenylamino)-4-(((((carboxymethyl)amino)carbonyl)methyl)amino)-
5-nitropyrimidine **514836-16-9P**, 2-(4-Chlorophenylamino)-4-
(carboxyphenylmethylamino)-5-nitropyrimidine **514836-17-0P**,
2-(4-Chlorophenylamino)-4-(((4'-hydroxybiphenyl-4-yl)methyl)amino)-5-
nitropyrimidine **514836-18-1P**, 2-(4-Chlorophenylamino)-4-(4-
hydroxybenzylamino)-5-nitropyrimidine **514836-20-5P**
514836-22-7P 514836-24-9P, 2-(4-Chlorophenylamino)-4-[(1-
(1H-benzimidazol-2-yl)ethyl)amino]-5-nitropyrimidine **514836-28-3P**
, 2-(4-Chlorophenylamino)-4-[N-methyl-N-(2-pyrazinylmethyl)amino]-5-
nitropyrimidine **514836-29-4P 514836-30-7P**,
2-(4-Chlorophenylamino)-4-[(4-(4-hydroxyphenyl)butyl)amino]-5-
nitropyrimidine **514836-32-9P**, 2-(4-Chlorophenylamino)-4-[((4-(2-
carboxyethyl)cyclohexyl)methyl)amino]-5-nitropyrimidine
514836-34-1P 514836-35-2P, 2-(4-Chlorophenylamino)-4-(3-
carboxybenzylamino)-5-nitropyrimidine **514836-36-3P**,
2-(4-Chlorophenylamino)-4-((6-tert-butoxycarbonylaminohexyl)amino)-5-
nitropyrimidine **514836-38-5P**, 2-(4-Chlorophenylamino)-4-((3-tert-
butoxycarbonylaminopropyl)amino)-5-nitropyrimidine **514836-40-9P**,
2-(4-Chlorophenylamino)-4-(4-carboxy-1-methyl-4-piperidinylamino)-5-
nitropyrimidine **514836-41-0P**, 2-(4-Chlorophenylamino)-4-[(1-
carboxy-2-(2-chlorophenyl)ethyl)amino]-5-nitropyrimidine
514836-43-2P 514836-44-3P, 2-(4-Chlorophenylamino)-4-[N-
((ethoxycarbonyl)methyl)-N-isopropylamino]-5-nitropyrimidine

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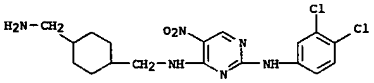
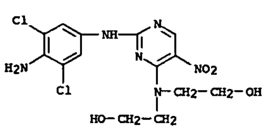
514836-45-4P, 2-(4-Chlorophenylamino)-4-
(((carbamimidoyl)methyl)amino)-5-nitropyrimidine **514836-46-5P**,
2-(4-Chlorophenylamino)-4-[(2-(6-methoxy-1H-benzimidazol-2-yl)ethyl)amino]-
5-nitropyrimidine **514836-47-6P**, 2-(4-Chlorophenylamino)-4-(2-
carboxybenzylamino)-5-nitropyrimidine **514836-49-8P**,
2-(4-Chlorophenylamino)-4-(((2-aminocarbonyl-1,3-dihydro-isoindol-5-
yl)methyl)amino)-5-nitropyrimidine **514836-51-2P**,
2-(4-Chlorophenylamino)-4-[((3-((tert-butoxycarbonylamino)methyl)cyclohexy
l)methyl)amino]-5-nitropyrimidine **514836-52-3P**
514836-55-6P, 2-(4-Chlorophenylamino)-4-(2-hydroxycyclohexylamino)-
5-nitropyrimidine **514836-58-9P**, 2-(4-Chlorophenylamino)-4-[N-
methyl-N-(2-pyridylmethyl)amino]-5-nitropyrimidine **514836-59-0P**,
2-(4-Chlorophenylamino)-4-[N-methyl-N-(3-pyridylmethyl)amino]-5-
nitropyrimidine **514836-60-3P**, 2-(4-Chlorophenylamino)-4-(1-ethyl-
3-piperidinylamino)-5-nitropyrimidine **514836-62-5P**,
2-(4-Chlorophenylamino)-4-(2-dimethylaminocyclohexylamino)-5-
nitropyrimidine **514836-66-9P**, 2-(4-Chlorophenylamino)-4-[N-
methyl-N-[3-(4-pyridyl)propyl]amino]-5-nitropyrimidine
514836-68-1P, 2-(4-Chlorophenylamino)-4-((4-dimethylamino-2-
phenylbutyl)amino)-5-nitropyrimidine **514836-72-7P**,
2-(4-Chlorophenylamino)-4-[bis-(3-pyridylmethyl)amino]-5-nitropyrimidine
514836-76-1P, 2-(4-Chlorophenylamino)-4-[(2-ethoxycarbonyl-1-(3-
pyridyl)ethyl)amino]-5-nitropyrimidine **514836-78-3P**,
2-(4-Chlorophenylamino)-4-[(1,1-dimethyl-3-(2-oxo-3-(pyridin-4-
yl)imidazolidin-1-yl)propyl)amino]-5-nitropyrimidine **514836-82-9P**
, 2-(4-Chlorophenylamino)-4-((2-cyanoethyl)amino)-5-nitropyrimidine
514836-85-2P
, 2-(3,4-Dichlorophenylamino)-4-[3-(dimethylamino)propylamino]-5-
nitropyrimidine **514836-87-4P**, 2-(3,4-Dichlorophenylamino)-4-(2-
hydroxyethylamino)-5-nitropyrimidine **514836-89-6P**,
2-(3,4-Dichlorophenylamino)-4-(2-methoxyethylamino)-5-nitropyrimidine
514836-90-9P, 2-(3,4-Dichlorophenylamino)-4-[2-
(dimethylamino)ethylamino]-5-nitropyrimidine **514836-92-1P**,
2-(3,4-Dichlorophenylamino)-4-(2-morpholinoethylamino)-5-nitropyrimidine
514836-94-3P, 2-(3,4-Dichlorophenylamino)-4-[4-
(dimethylamino)butylamino]-5-nitropyrimidine **514836-98-7P**,
2-(4-Chlorophenylamino)-4-[(2-(methylsulfonylamino)ethyl)amino]-5-
nitropyrimidine **514837-00-4P**, 2-(4-Chlorophenylamino)-4-
(carboxymethylamino)-5-nitropyrimidine **514837-01-5P**,
2-(3,4-Dichlorophenylamino)-4-[(2-carboxyethyl)amino]-5-nitropyrimidine
514837-78-6P 514837-88-8P, 2-(1-Naphthylamino)-4-[N-
(trans-4-hydroxycyclohexyl)-N-methylamino]-5-nitropyrimidine
514838-05-2P, 2-((4-Morpholinophenyl)amino)-4-(2-
acetylaminoethylamino)-5-nitropyrimidine **514838-07-4P**,
2-[(4-(N-Methyl-N-methylsulfonylamino)phenyl)amino]-4-[N-(trans-4-
hydroxycyclohexyl)-N-methylamino]-5-nitropyrimidine **514838-08-5P**
, 2-((4-(N,N-Diethylaminomethyl)phenyl)amino)-4-(2-acetylaminoethylamino)-
5-nitropyrimidine **514838-09-6P**, 2-(1,3-Dihydro-2-oxoindol-6-
ylamino)-4-[N-(trans-4-hydroxycyclohexyl)-N-methylamino]-5-nitropyrimidine
514838-11-0P, 2-[(4-(N-Methyl-N-methylsulfonylamino)phenyl)amino]-
4-(2-acetylaminoethylamino)-5-nitropyrimidine **514838-15-4P**,
2-(3-Hydroxy-4-methylphenylamino)-4-[N-(trans-4-hydroxycyclohexyl)-N-
methylamino]-5-nitropyrimidine **514838-16-5P**,
2-(6-Indazolylamino)-4-[N-(trans-4-hydroxycyclohexyl)-N-methylamino]-5-
nitropyrimidine **514838-18-7P**, 2-[(4-(3-
Diethylaminopropoxy)phenyl)amino]-4-(2-pyridylmethylamino)-5-
nitropyrimidine **514838-22-3P**, 2-((4-
(Benzylaminocarbonyl)phenyl)amino)-4-[N-(2-hydroxyethyl)-N-methylamino]-5-
nitropyrimidine **514838-23-4P**, 2-(3-Carboxyphenylamino)-4-[N-
(trans-4-hydroxycyclohexyl)-N-methylamino]-5-nitropyrimidine
514838-25-6P, 2-(5-Carboxy-2-naphthylamino)-4-(2-
acetylaminoethylamino)-5-nitropyrimidine **514838-26-7P**,

L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
2-(5-Carboxy-2-naphthylamino)-4-(ethoxycarbonylmethylamino)-5-
nitropyrimidine **514838-27-8P**, 2-((4-
(Phenylaminocarbonyl)phenyl)amino)-4-[N-(2-hydroxyethyl)-N-methylamino]-5-
nitropyrimidine **514838-29-0P**, 2-[(4-(4-Methyl-1-
piperazinyl)phenyl)amino]-4-[N-(trans-4-hydroxycyclohexyl)-N-methylamino]-
5-nitropyrimidine **514843-25-5P**, 2-(3,4-Dichlorophenylamino)-4-(2-
acetylaminoethylamino)-5-nitropyrimidine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(drug candidate; prepn. of trisubstituted pyrimidines as cyclin
dependent kinase inhibitors)

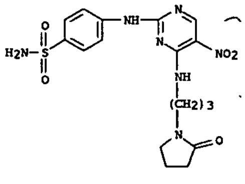
RN 514830-60-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)cyclohexyl]methyl]-N2-(3,4-
dichlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)



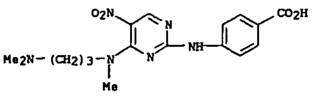
RN 514830-66-1 HCAPLUS
CN Ethanol, 2,2'-[[2-[(4-amino-3,5-dichlorophenyl)amino]-5-nitro-4-
pyrimidinyl]imino]bis- (9CI) (CA INDEX NAME)



RN 514830-67-2 HCAPLUS
CN Benzenesulfonamide, 4-[[5-nitro-4-[[3-(2-oxo-1-pyrrolidinyl)propyl]amino]-
2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



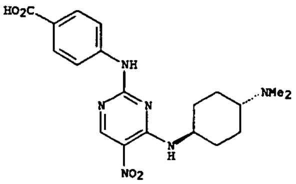
RN 514830-72-9 HCAPLUS
CN Benzoic acid, 4-[[4-[[3-(dimethylamino)propyl]methylamino]-5-nitro-2-
pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 514830-77-4 HCAPLUS

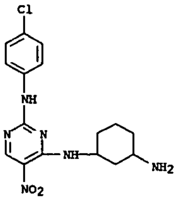
CN Benzoic acid, 4-[[4-[[trans-4-(dimethylamino)cyclohexyl]amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



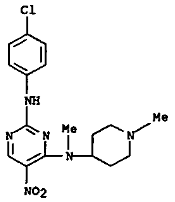
RN 514830-93-4 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-(3-aminocyclohexyl)-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)



RN 514831-03-9 HCAPLUS

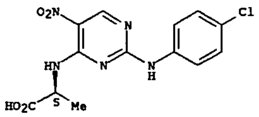
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-methyl-N4-(1-methyl-4-piperidinyl)-5-nitro- (9CI) (CA INDEX NAME)



RN 514831-07-3 HCAPLUS

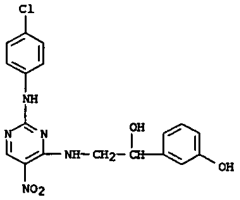
CN L-Alanine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



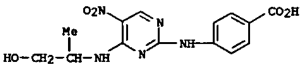
RN 514831-18-6 HCAPLUS

CN Benzenemethanol, α-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]-3-hydroxy- (9CI) (CA INDEX NAME)



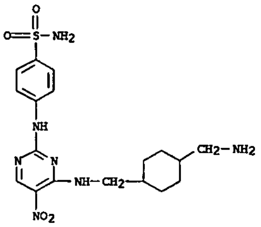
RN 514831-34-6 HCAPLUS

CN Benzoic acid, 4-[[4-[(2-hydroxy-1-methylethyl)amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



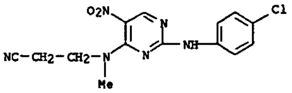
RN 514831-35-7 HCAPLUS

CN Benzenesulfonamide, 4-[[4-[[[4-(aminomethyl)cyclohexyl]methyl]amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



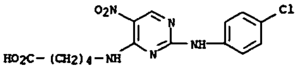
RN 514831-42-6 HCAPLUS

CN Propanenitrile, 3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]methylamino]- (9CI) (CA INDEX NAME)



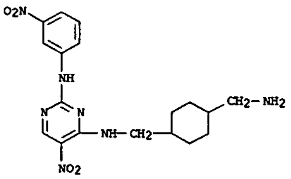
RN 514831-46-0 HCAPLUS

CN Pentanoic acid, 5-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



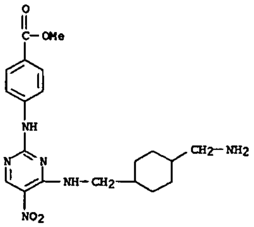
RN 514831-52-8 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)cyclohexyl]methyl]-5-nitro-N2-(3-nitrophenyl)- (9CI) (CA INDEX NAME)



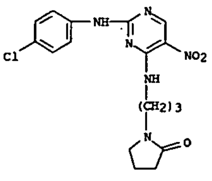
RN 514831-54-0 HCAPLUS

CN Benzoic acid, 4-[[4-[[[4-(aminomethyl)cyclohexyl]methyl]amino]-5-nitro-2-pyrimidinyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



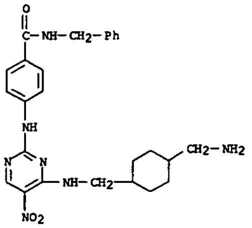
RN 514831-55-1 HCAPLUS

CN 2-Pyrrolidinone, 1-[3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]propyl]- (9CI) (CA INDEX NAME)

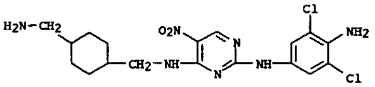


RN 514831-58-4 HCAPLUS

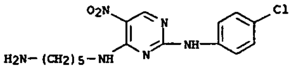
CN Benzamide, 4-[[4-[[[4-(aminomethyl)cyclohexyl]methyl]amino]-5-nitro-2-pyrimidinyl]amino]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



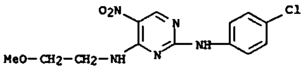
RN 514831-60-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-amino-3,5-dichlorophenyl)-N4-[[4-(aminomethyl)cyclohexyl]methyl]-5-nitro- (9CI) (CA INDEX NAME)



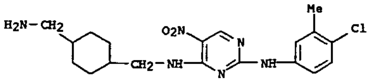
RN 514831-66-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-(5-aminopentyl)-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)



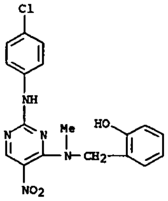
RN 514831-70-0 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-(2-methoxyethyl)-5-nitro- (9CI) (CA INDEX NAME)



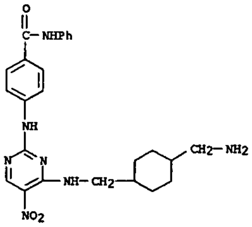
RN 514831-75-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)cyclohexyl]methyl]-N2-(4-chloro-3-methylphenyl)-5-nitro- (9CI) (CA INDEX NAME)



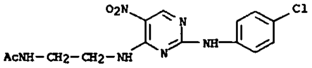
RN 514831-82-4 HCAPLUS
CN Phenol, 2-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]methylamino]methyl]- (9CI) (CA INDEX NAME)



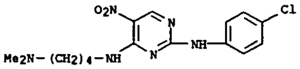
RN 514831-83-5 HCAPLUS
CN Benzamide, 4-[[4-[[[4-(aminomethyl)cyclohexyl]methyl]amino]-5-nitro-2-pyrimidinyl]amino]-N-phenyl- (9CI) (CA INDEX NAME)



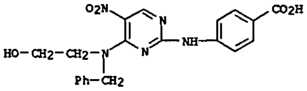
RN 514832-09-8 HCAPLUS
CN Acetamide, N-[2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)



RN 514832-11-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[4-(dimethylamino)butyl]-5-nitro- (9CI) (CA INDEX NAME)

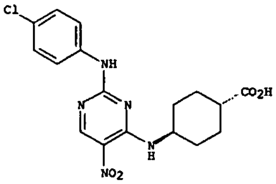


RN 514832-14-5 HCAPLUS
CN Benzoic acid, 4-[[4-[(2-hydroxyethyl)(phenylmethyl)amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

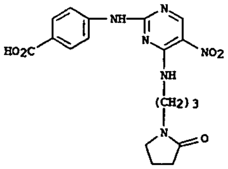


RN 514832-18-9 HCAPLUS
CN Cyclohexanecarboxylic acid, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-, trans- (9CI) (CA INDEX NAME)

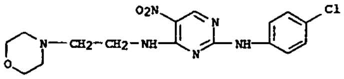
Relative stereochemistry.



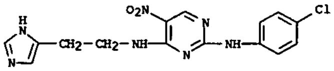
RN 514832-20-3 HCAPLUS
CN Benzoic acid, 4-[[5-nitro-4-[[3-(2-oxo-1-pyrrolidinyl)propyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



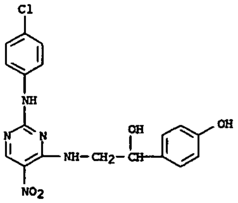
RN 514832-21-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(4-morpholinyl)ethyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 514832-23-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(1H-imidazol-4-yl)ethyl]-5-nitro- (9CI) (CA INDEX NAME)

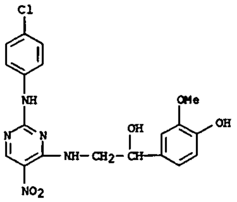


RN 514832-24-7 HCAPLUS
CN Benzenemethanol, α-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]-4-hydroxy- (9CI) (CA INDEX NAME)

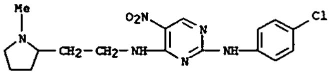


RN 514832-25-8 HCAPLUS
CN Benzenemethanol, α-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-

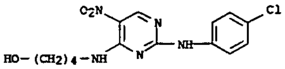
pyrimidinyl]amino]methyl]-4-hydroxy-3-methoxy- (9CI) (CA INDEX NAME)



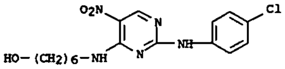
RN 514832-26-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(1-methyl-2-pyrrolidinyl)ethyl]-5-nitro- (9CI) (CA INDEX NAME)



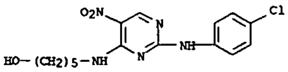
RN 514832-27-0 HCAPLUS
CN 1-Butanol, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



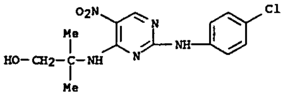
RN 514832-28-1 HCAPLUS
CN 1-Hexanol, 6-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



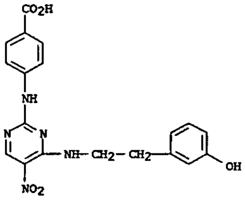
RN 514832-29-2 HCAPLUS
CN 1-Pentanol, 5-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



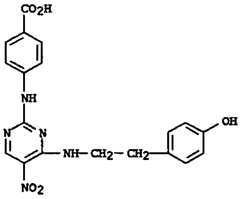
RN 514832-30-5 HCAPLUS
CN 1-Propanol, 2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-2-methyl- (9CI) (CA INDEX NAME)



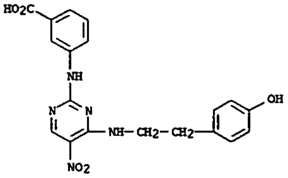
RN 514832-31-6 HCAPLUS
CN Benzoic acid, 4-[[4-[[2-(3-hydroxyphenyl)ethyl]amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



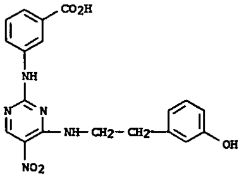
RN 514832-34-9 HCAPLUS
CN Benzoic acid, 4-[[4-[[2-(4-hydroxyphenyl)ethyl]amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



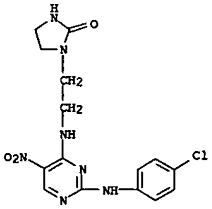
RN 514832-36-1 HCAPLUS
CN Benzoic acid, 3-[[4-[[2-(4-hydroxyphenyl)ethyl]amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



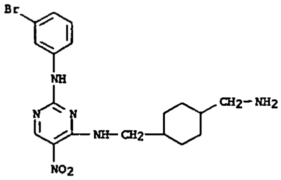
RN 514832-37-2 HCAPLUS
CN Benzoic acid, 3-[[4-[[2-(3-hydroxyphenyl)ethyl]amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



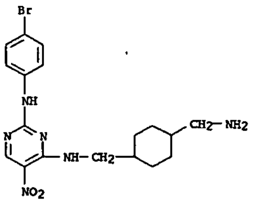
RN 514832-38-3 HCAPLUS
CN 2-Imidazolidinone, 1-[2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)



RN 514832-40-7 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)cyclohexyl]methyl]-N2-(3-bromophenyl)-5-nitro- (9CI) (CA INDEX NAME)

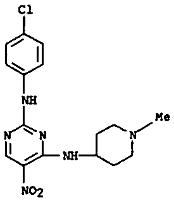


RN 514832-41-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)cyclohexyl]methyl]-N2-(4-bromophenyl)-5-nitro- (9CI) (CA INDEX NAME)

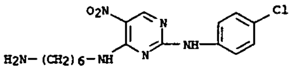


RN 514832-42-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-(1-methyl-4-piperidinyl)-5-nitro- (9CI) (CA INDEX NAME)

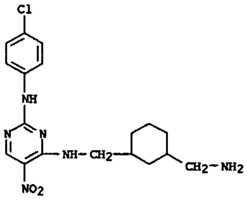
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 514832-43-0 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-(6-aminohexyl)-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)

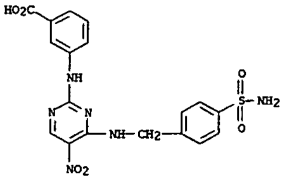


RN 514832-44-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[[3-(aminomethyl)cyclohexyl]methyl]-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)

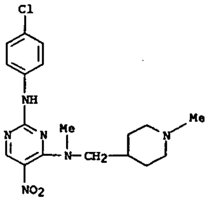


RN 514832-46-3 HCAPLUS
CN Benzoic acid, 3-[[4-[[[4-(aminosulfonyl)phenyl]methyl]amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

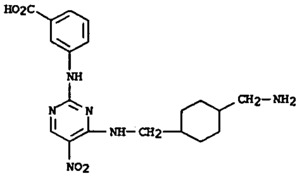
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 514832-47-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-methyl-N4-[(1-methyl-4-piperidinyl)methyl]-5-nitro- (9CI) (CA INDEX NAME)

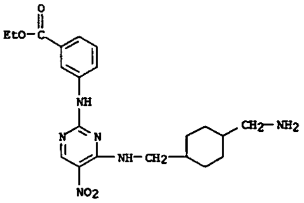


RN 514832-48-5 HCAPLUS
CN Benzoic acid, 3-[[4-[[[4-(aminomethyl)cyclohexyl]methyl]amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

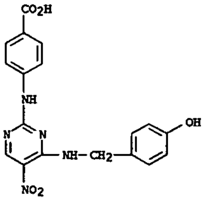


RN 514832-49-6 HCAPLUS
CN Benzoic acid, 3-[[4-[[[4-(aminomethyl)cyclohexyl]methyl]amino]-5-nitro-2-pyrimidinyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

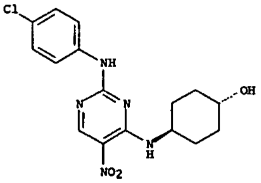


RN 514832-53-2 HCAPLUS
CN Benzoic acid, 4-[[4-[[(4-hydroxyphenyl)methyl]amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



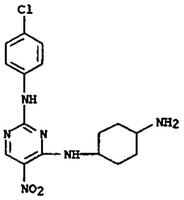
RN 514832-59-8 HCAPLUS
CN Cyclohexanol, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

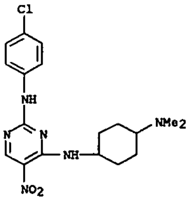


RN 514832-60-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-(4-aminocyclohexyl)-N2-(4-chlorophenyl)-5-nitro-

L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(9CI) (CA INDEX NAME)

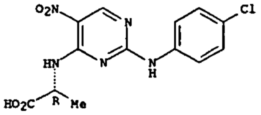


RN 514832-61-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[4-(dimethylamino)cyclohexyl]-5-nitro- (9CI) (CA INDEX NAME)



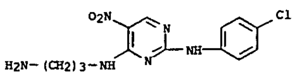
RN 514832-62-3 HCAPLUS
CN D-Alanine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

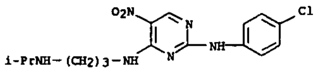


RN 514832-63-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-(3-aminopropyl)-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)

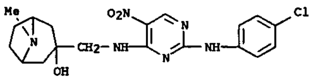
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



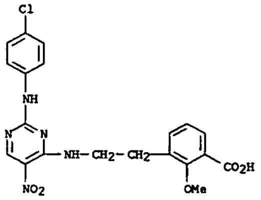
RN 514832-64-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[3-[(1-methylethyl)amino]propyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 514832-65-6 HCAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-ol, 3-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]-8-methyl- (9CI) (CA INDEX NAME)

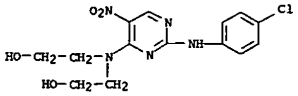


RN 514832-66-7 HCAPLUS
CN Benzoic acid, 3-[2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethyl]-2-methoxy- (9CI) (CA INDEX NAME)

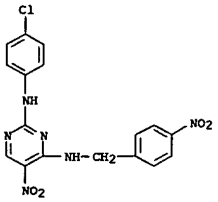


RN 514832-68-9 HCAPLUS
CN Ethanol, 2,2'-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]imino]bis- (9CI) (CA INDEX NAME)

L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

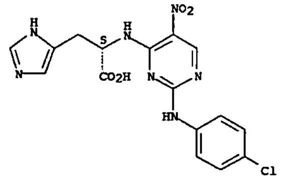


RN 514832-69-0 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[(4-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)



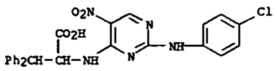
RN 514832-70-3 HCAPLUS
CN L-Histidine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

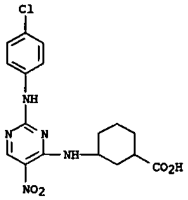


RN 514832-71-4 HCAPLUS
CN Phenylalanine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]-β-phenyl- (9CI) (CA INDEX NAME)

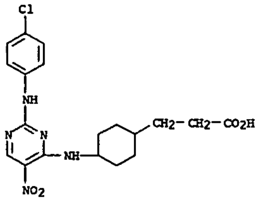
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 514832-72-5 HCAPLUS
CN Cyclohexanecarboxylic acid, 3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

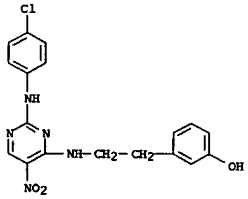


RN 514832-73-6 HCAPLUS
CN Cyclohexanepropanoic acid, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

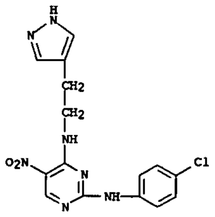


RN 514832-74-7 HCAPLUS
CN Phenol, 3-[2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

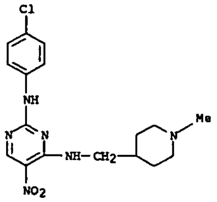
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 514832-75-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[2-(1H-pyrazol-4-yl)ethyl]- (9CI) (CA INDEX NAME)



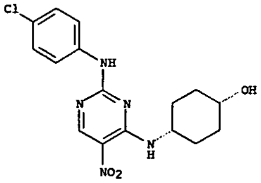
RN 514832-76-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[(1-methyl-4-piperidinyl)methyl]-5-nitro- (9CI) (CA INDEX NAME)



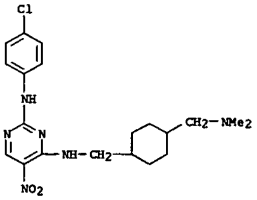
RN 514832-77-0 HCAPLUS
CN Cyclohexanol, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-,

L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

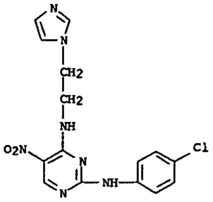


RN 514832-78-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[[4-[(dimethylamino)methyl]cyclohexyl]methyl]-5-nitro- (9CI) (CA INDEX NAME)

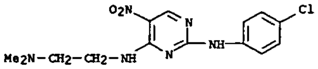


RN 514832-79-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(1H-imidazol-1-yl)ethyl]-5-nitro- (9CI) (CA INDEX NAME)

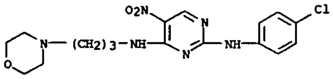
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



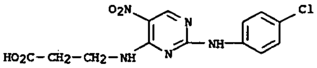
RN 514834-74-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(dimethylamino)ethyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 514834-75-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[3-(4-morpholinyl)propyl]-5-nitro- (9CI) (CA INDEX NAME)

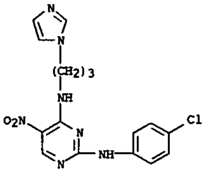


RN 514834-76-5 HCAPLUS
CN β-Alanine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

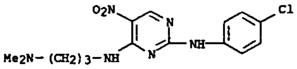


RN 514834-77-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[3-(1H-imidazol-1-yl)propyl]-5-nitro- (9CI) (CA INDEX NAME)

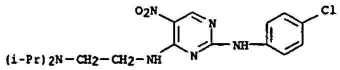
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



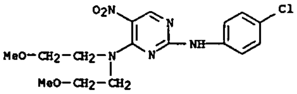
RN 514834-78-7 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[3-(dimethylamino)propyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 514834-79-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[2-[bis(1-methylethyl)amino]ethyl]-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)

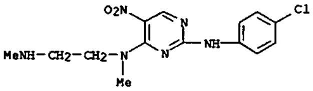


RN 514834-80-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4,N4-bis(2-methoxyethyl)-5-nitro- (9CI) (CA INDEX NAME)

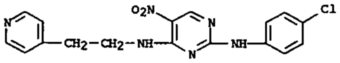


RN 514834-81-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-methyl-N4-[2-(methylamino)ethyl]-5-nitro- (9CI) (CA INDEX NAME)

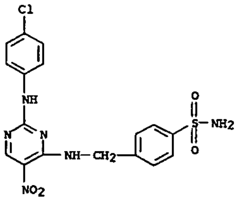
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



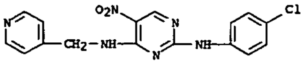
RN 514834-82-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



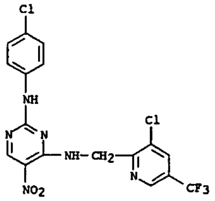
RN 514834-83-4 HCAPLUS
CN Benzenesulfonamide, 4-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



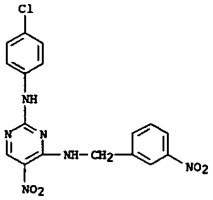
RN 514834-84-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



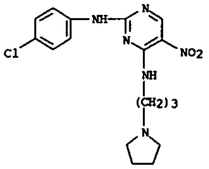
RN 514834-85-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[[3-chloro-5-(trifluoromethyl)-2-pyridinyl]methyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 514834-86-7 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[(3-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)



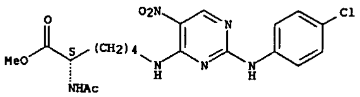
RN 514834-88-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[3-(1-pyrrolidinyl)propyl]- (9CI) (CA INDEX NAME)



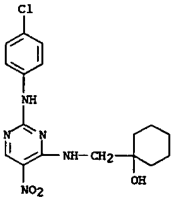
RN 514834-89-0 HCAPLUS

CN L-Lysine, N2-acetyl-N6-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]-, methyl ester (9CI) (CA INDEX NAME)

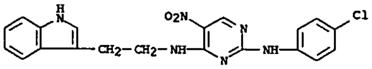
Absolute stereochemistry.



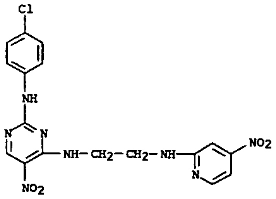
RN 514834-90-3 HCAPLUS
CN Cyclohexanol, 1-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



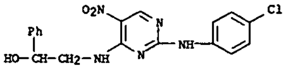
RN 514834-91-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(1H-indol-3-yl)ethyl]-5-nitro- (9CI) (CA INDEX NAME)



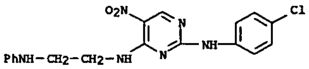
RN 514834-92-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[2-[(4-nitro-2-pyridinyl)amino]ethyl]- (9CI) (CA INDEX NAME)



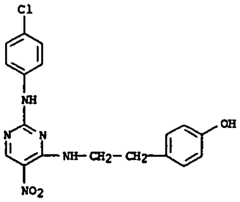
RN 514834-93-6 HCAPLUS
CN Benzenemethanol, α-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



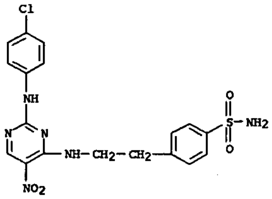
RN 514834-94-7 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[2-(phenylamino)ethyl]- (9CI) (CA INDEX NAME)



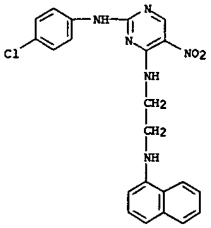
RN 514834-95-8 HCAPLUS
CN Phenol, 4-[2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)



RN 514834-96-9 HCAPLUS
CN Benzenesulfonamide, 4-[2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

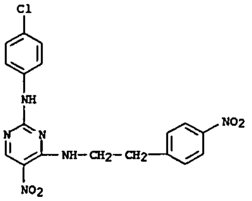


RN 514834-97-0 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(1-naphthalenylamino)ethyl]-5-nitro- (9CI) (CA INDEX NAME)

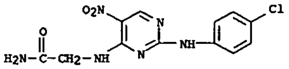


RN 514834-98-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[2-(4-nitrophenyl)ethyl]- (9CI) (CA INDEX NAME)

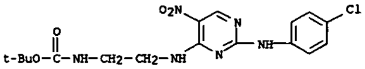
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



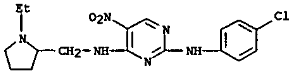
RN 514835-00-8 HCAPLUS
CN Acetamide, 2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 514835-04-2 HCAPLUS
CN Carbamic acid, [2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

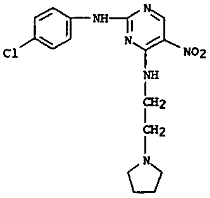


RN 514835-05-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[(1-ethyl-2-pyrrolidinyl)methyl]-5-nitro- (9CI) (CA INDEX NAME)

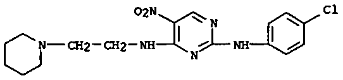


RN 514835-07-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[2-(1-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)

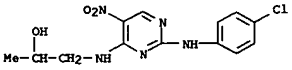
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



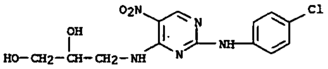
RN 514835-08-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)



RN 514835-09-7 HCAPLUS
CN 2-Propanol, 1-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

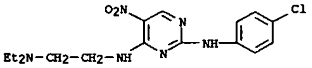


RN 514835-10-0 HCAPLUS
CN 1,2-Propanediol, 3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

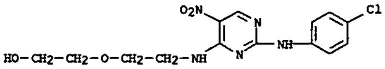


RN 514835-11-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(diethylamino)ethyl]-5-nitro- (9CI) (CA INDEX NAME)

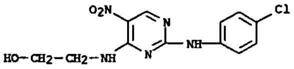
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



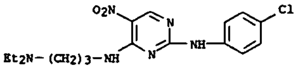
RN 514835-12-2 HCAPLUS
CN Ethanol, 2-[2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethoxy]- (9CI) (CA INDEX NAME)



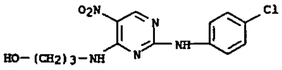
RN 514835-13-3 HCAPLUS
CN Ethanol, 2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 514835-14-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[3-(diethylamino)propyl]-5-nitro- (9CI) (CA INDEX NAME)

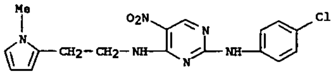


RN 514835-15-5 HCAPLUS
CN 1-Propanol, 3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

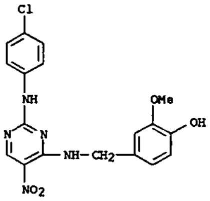


RN 514835-16-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(1-methyl-1H-pyrrol-2-yl)ethyl]-5-nitro- (9CI) (CA INDEX NAME)

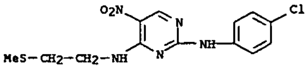
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



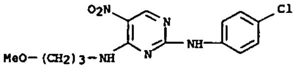
RN 514835-17-7 HCAPLUS
CN Phenol, 4-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]-2-methoxy- (9CI) (CA INDEX NAME)



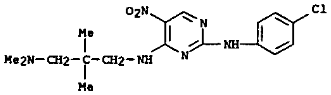
RN 514835-18-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(methylthio)ethyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 514835-19-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-(3-methoxypropyl)-5-nitro- (9CI) (CA INDEX NAME)

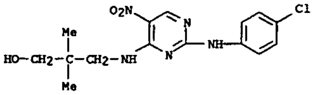


RN 514835-21-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[3-(dimethylamino)-2,2-dimethylpropyl]-5-nitro- (9CI) (CA INDEX NAME)



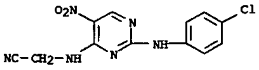
RN 514835-22-4 HCAPLUS

CN 1-Propanol, 3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-2,2-dimethyl- (9CI) (CA INDEX NAME)



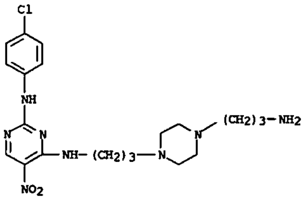
RN 514835-23-5 HCAPLUS

CN Acetonitrile, [[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 514835-35-9 HCAPLUS

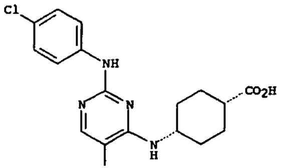
CN 2,4-Pyrimidinediamine, N4-[3-[4-(3-aminopropyl)-1-piperazinyl]propyl]-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)



RN 514835-37-1 HCAPLUS

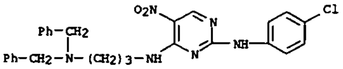
CN Cyclohexanecarboxylic acid, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



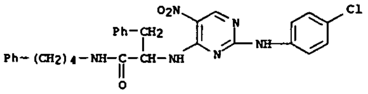
RN 514835-39-3 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-[3-[bis(phenylmethyl)amino]propyl]-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)



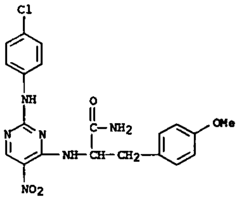
RN 514835-41-7 HCAPLUS

CN Benzenepropanamide, α-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-N-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



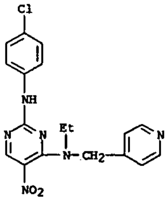
RN 514835-43-9 HCAPLUS

CN Benzenepropanamide, α-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-4-methoxy- (9CI) (CA INDEX NAME)



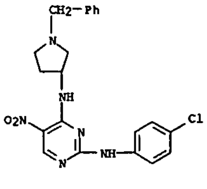
RN 514835-45-1 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-ethyl-5-nitro-N4-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



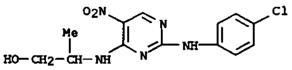
RN 514835-55-3 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[1-(phenylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)



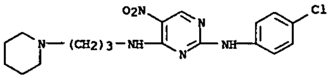
RN 514835-56-4 HCAPLUS

CN 1-Propanol, 2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



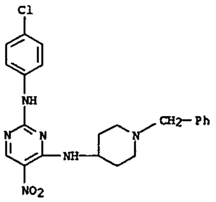
RN 514835-57-5 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[3-(1-piperidinyl)propyl]- (9CI) (CA INDEX NAME)



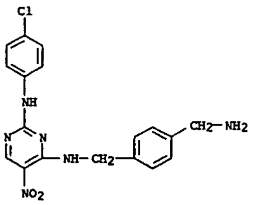
RN 514835-58-6 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[1-(phenylmethyl)-4-piperidinyl]- (9CI) (CA INDEX NAME)



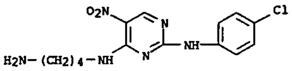
RN 514835-59-7 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-[[4-(aminomethyl)phenyl]methyl]-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)

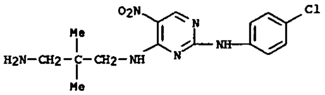


RN 514835-60-0 HCAPLUS

L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 2,4-Pyrimidinediamine, N4-(4-aminobutyl)-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)

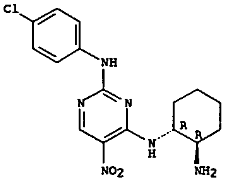


RN 514835-61-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-(3-amino-2,2-dimethylpropyl)-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)

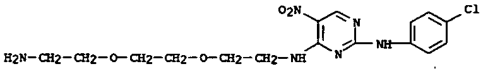


RN 514835-62-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[(1R,2R)-2-aminocyclohexyl]-N2-(4-chlorophenyl)-5-nitro-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

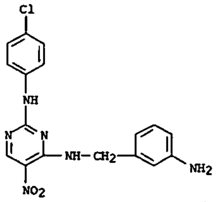


RN 514835-63-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[2-[2-(2-aminoethoxy)ethoxy]ethyl]-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)

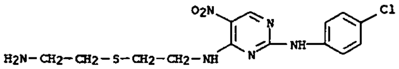


RN 514835-64-4 HCAPLUS

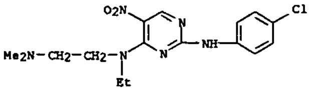
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 2,4-Pyrimidinediamine, N4-[(3-aminophenyl)methyl]-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)



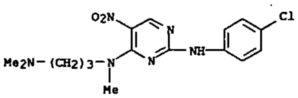
RN 514835-65-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[2-[(2-aminoethyl)thio]ethyl]-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)



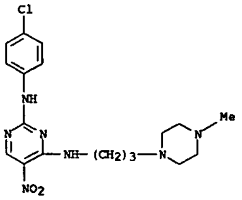
RN 514835-66-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(dimethylamino)ethyl]-N4-ethyl-5-nitro- (9CI) (CA INDEX NAME)



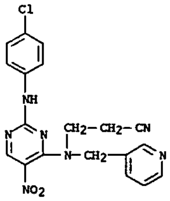
RN 514835-67-7 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[3-(dimethylamino)propyl]-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



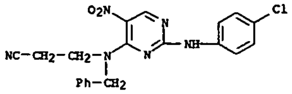
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 514835-68-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[3-(4-methyl-1-piperazinyl)propyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 514835-69-9 HCAPLUS
CN Propanenitrile, 3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl](3-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)

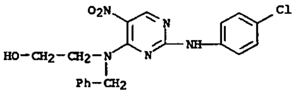


RN 514835-72-4 HCAPLUS
CN Propanenitrile, 3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl](phenylmethyl)amino]- (9CI) (CA INDEX NAME)

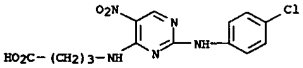


RN 514835-73-5 HCAPLUS
CN Ethanol, 2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl](phenylmethyl)amino]- (9CI) (CA INDEX NAME)

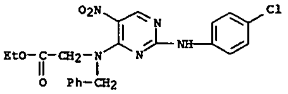
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



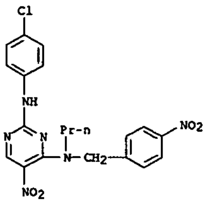
RN 514835-74-6 HCAPLUS
CN Butanoic acid, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



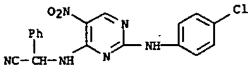
RN 514835-75-7 HCAPLUS
CN Glycine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]-N-(phenylmethyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 514835-76-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-[(4-nitrophenyl)methyl]-N4-propyl- (9CI) (CA INDEX NAME)

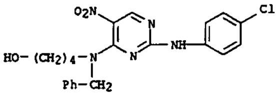


RN 514835-78-0 HCAPLUS
CN Benzeneacetonitrile, α-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



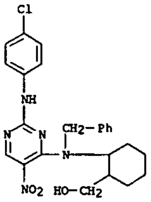
RN 514835-79-1 HCAPLUS

CN 1-Butanol, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl](phenylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 514835-80-4 HCAPLUS

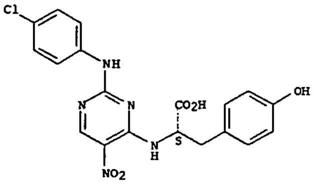
CN Cyclohexanemethanol, 2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl](phenylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 514835-81-5 HCAPLUS

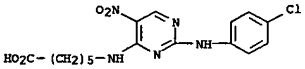
CN L-Tyrosine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 514835-82-6 HCAPLUS

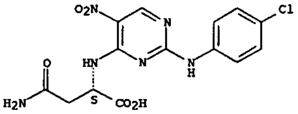
CN Hexanoic acid, 6-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 514835-83-7 HCAPLUS

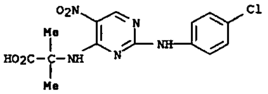
CN L-Asparagine, N2-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 514835-84-8 HCAPLUS

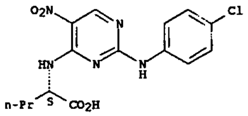
CN Alanine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]-2-methyl- (9CI) (CA INDEX NAME)



RN 514835-85-9 HCAPLUS

CN L-Norvaline, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

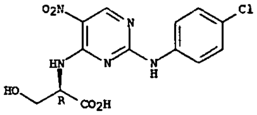
Absolute stereochemistry.



RN 514835-86-0 HCAPLUS

CN D-Serine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

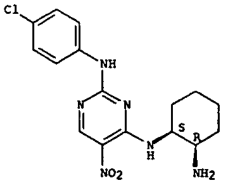
Absolute stereochemistry.



RN 514835-88-2 HCAPLUS

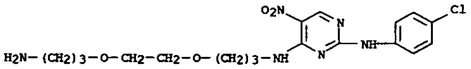
CN 2,4-Pyrimidinediamine, N4-[(1R,2S)-2-aminocyclohexyl]-N2-(4-chlorophenyl)-5-nitro-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



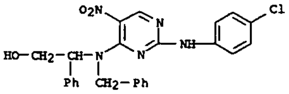
RN 514835-92-8 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-[3-[2-(3-aminopropoxy)ethoxy]propyl]-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)



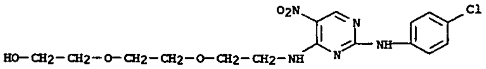
RN 514835-93-9 HCAPLUS

CN Benzeneethanol, β-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl](phenylmethyl)amino]- (9CI) (CA INDEX NAME)



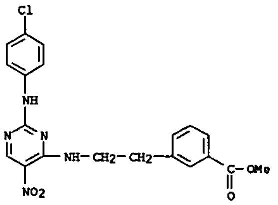
RN 514835-95-1 HCAPLUS

CN Ethanol, 2-[2-[2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethoxy]ethoxy]- (9CI) (CA INDEX NAME)



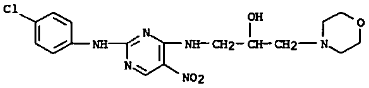
RN 514835-96-2 HCAPLUS

CN Benzoic acid, 3-[2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

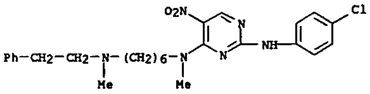


RN 514835-97-3 HCAPLUS

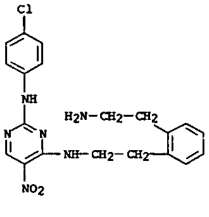
CN 4-Morpholineethanol, α-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



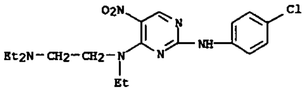
RN 514835-98-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-methyl-N4-[6-[methyl(2-phenylethyl)amino]hexyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 514835-99-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[2-[2-(2-aminoethyl)phenyl]ethyl]-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)

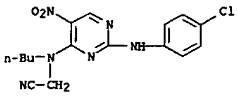


RN 514836-00-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(diethylamino)ethyl]-N4-ethyl-5-nitro- (9CI) (CA INDEX NAME)

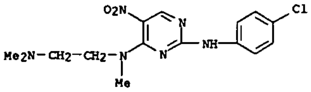


RN 514836-03-4 HCAPLUS
CN Acetonitrile, [butyl[2-[(4-chlorophenyl)amino]-5-nitro-4-

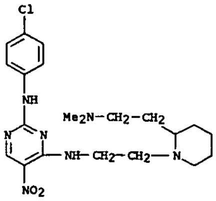
pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



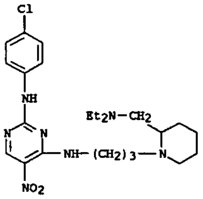
RN 514836-04-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(dimethylamino)ethyl]-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



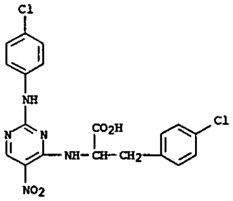
RN 514836-11-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-[2-(dimethylamino)ethyl]-1-piperidinyl]ethyl]-5-nitro- (9CI) (CA INDEX NAME)



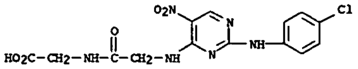
RN 514836-12-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[3-[2-[(diethylamino)methyl]-1-piperidinyl]propyl]-5-nitro- (9CI) (CA INDEX NAME)



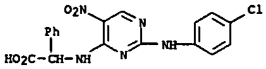
RN 514836-14-7 HCAPLUS
CN Phenylalanine, 4-chloro-N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



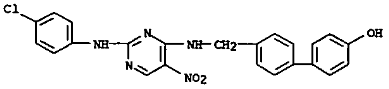
RN 514836-15-8 HCAPLUS
CN Glycine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]glycyl- (9CI) (CA INDEX NAME)



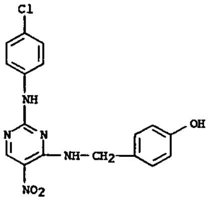
RN 514836-16-9 HCAPLUS
CN Benzeneacetic acid, α-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 514836-17-0 HCAPLUS
CN [1,1'-Biphenyl]-4-ol, 4'-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

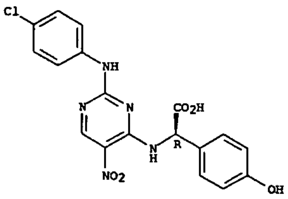


RN 514836-18-1 HCAPLUS
CN Phenol, 4-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



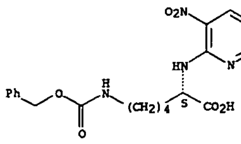
RN 514836-20-5 HCAPLUS
CN Benzeneacetic acid, α-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-4-hydroxy-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

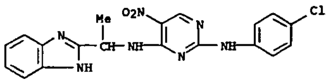


RN 514836-22-7 HCAPLUS
CN L-Lysine, N2-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]-N6-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

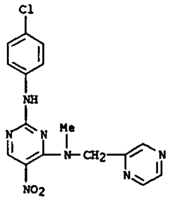
Absolute stereochemistry.



RN 514836-24-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[1-(1H-benzimidazol-2-yl)ethyl]-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)

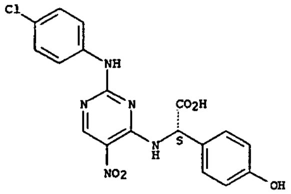


RN 514836-28-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-methyl-5-nitro-N4-(pyrazinylmethyl)- (9CI) (CA INDEX NAME)

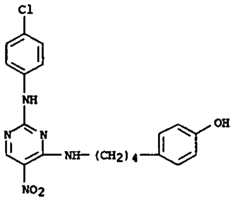


RN 514836-29-4 HCAPLUS
CN Benzeneacetic acid, α-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-4-hydroxy-, (αS)- (9CI) (CA INDEX NAME)

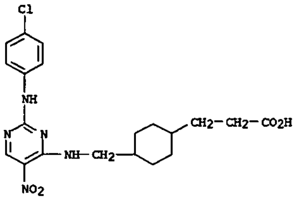
Absolute stereochemistry.



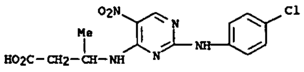
RN 514836-30-7 HCAPLUS
CN Phenol, 4-[4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]butyl]- (9CI) (CA INDEX NAME)



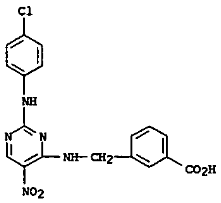
RN 514836-32-9 HCAPLUS
CN Cyclohexanepropanoic acid, 4-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



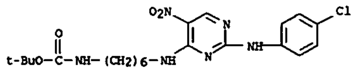
RN 514836-34-1 HCAPLUS
CN Butanoic acid, 3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



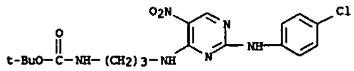
RN 514836-35-2 HCAPLUS
CN Benzoic acid, 3-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



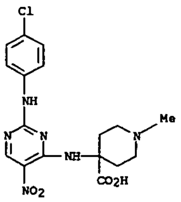
RN 514836-36-3 HCAPLUS
CN Carbamic acid, [6-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]hexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



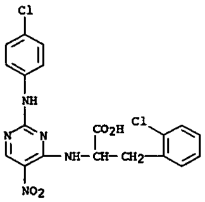
RN 514836-38-5 HCAPLUS
CN Carbamic acid, [3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 514836-40-9 HCAPLUS
CN 4-Piperidinecarboxylic acid, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-1-methyl- (9CI) (CA INDEX NAME)

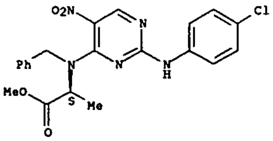


RN 514836-41-0 HCAPLUS
CN Phenylalanine, 2-chloro-N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

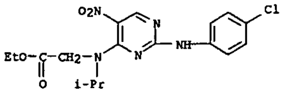


RN 514836-43-2 HCAPLUS
CN L-Alanine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]-N-(phenylmethyl)-, methyl ester (9CI) (CA INDEX NAME)

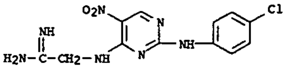
Absolute stereochemistry.



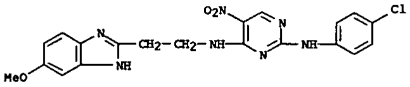
RN 514836-44-3 HCAPLUS
CN Glycine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]-N-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)



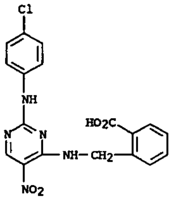
RN 514836-45-4 HCAPLUS
CN Ethanimidamide, 2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



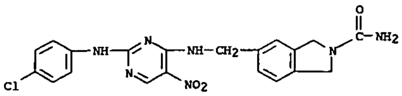
RN 514836-46-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(5-methoxy-1H-benzimidazol-2-yl)ethyl]-5-nitro- (9CI) (CA INDEX NAME)



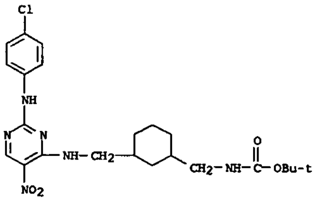
RN 514836-47-6 HCAPLUS
CN Benzoic acid, 2-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



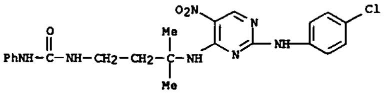
RN 514836-49-8 HCAPLUS
CN 2H-Isoindole-2-carboxamide, 5-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]-1,3-dihydro- (9CI) (CA INDEX NAME)



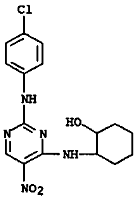
RN 514836-51-2 HCAPLUS
CN Carbamic acid, [[3-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



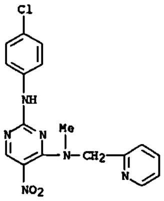
RN 514836-52-3 HCAPLUS
CN Urea, N-[3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-3-methylbutyl]-N'-phenyl- (9CI) (CA INDEX NAME)



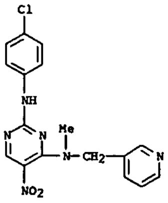
RN 514836-55-6 HCAPLUS
CN Cyclohexanol, 2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



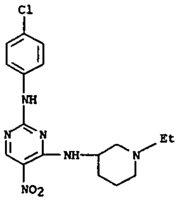
RN 514836-58-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-methyl-5-nitro-N4-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



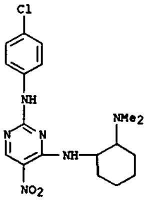
RN 514836-59-0 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-methyl-5-nitro-N4-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)



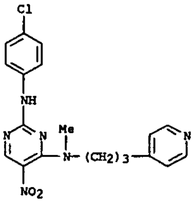
RN 514836-60-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-(1-ethyl-3-piperidinyl)-5-nitro- (9CI) (CA INDEX NAME)



RN 514836-62-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(dimethylamino)cyclohexyl]-5-nitro- (9CI) (CA INDEX NAME)

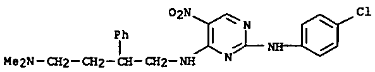


RN 514836-66-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-methyl-5-nitro-N4-[3-(4-pyridinyl)propyl]- (9CI) (CA INDEX NAME)

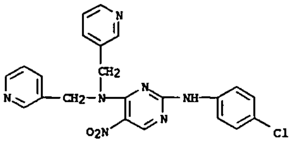


RN 514836-68-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[4-(dimethylamino)-2-

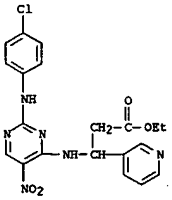
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
phenylbutyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 514836-72-7 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4,N4-bis(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

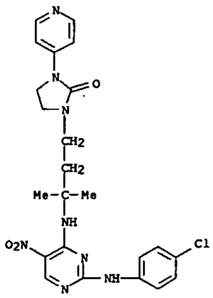


RN 514836-76-1 HCAPLUS
CN 3-Pyridinepropanoic acid, β-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

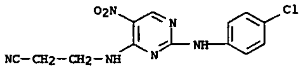


RN 514836-78-3 HCAPLUS
CN 2-Imidazolidinone, 1-[3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-3-methylbutyl]-3-(4-pyridinyl)- (9CI) (CA INDEX NAME)

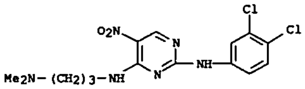
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 514836-82-9 HCAPLUS
CN Propanenitrile, 3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

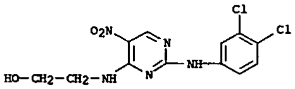


RN 514836-85-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-[3-(dimethylamino)propyl]-5-nitro- (9CI) (CA INDEX NAME)

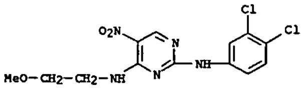


RN 514836-87-4 HCAPLUS
CN Ethanol, 2-[[2-[(3,4-dichlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

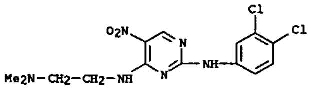
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



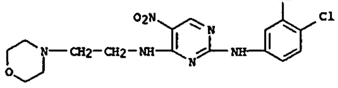
RN 514836-89-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-(2-methoxyethyl)-5-nitro- (9CI) (CA INDEX NAME)



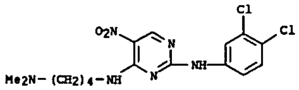
RN 514836-90-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-[2-(dimethylamino)ethyl]-5-nitro- (9CI) (CA INDEX NAME)



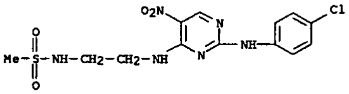
RN 514836-92-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-[2-(4-morpholinyl)ethyl]-5-nitro- (9CI) (CA INDEX NAME)



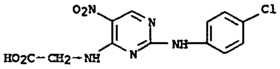
RN 514836-94-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-[4-(dimethylamino)butyl]-5-nitro- (9CI) (CA INDEX NAME)



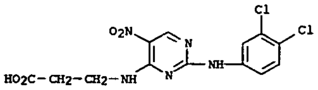
L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 514836-98-7 HCAPLUS
CN Methanesulfonamide, N-[2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)



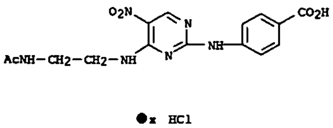
RN 514837-00-4 HCAPLUS
CN Glycine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 514837-01-5 HCAPLUS
CN β-Alanine, N-[2-[(3,4-dichlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

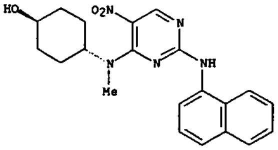


RN 514837-78-6 HCAPLUS
CN Benzoic acid, 4-[[4-[[2-(acetylamino)ethyl]amino]-5-nitro-2-pyrimidinyl]amino]-, hydrochloride (9CI) (CA INDEX NAME)

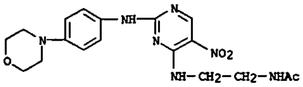


RN 514837-88-8 HCAPLUS
CN Cyclohexanol, 4-[methyl[2-(1-naphthalenylamino)-5-nitro-4-pyrimidinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

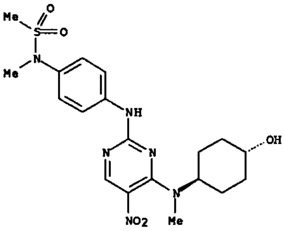


RN 514838-05-2 HCAPLUS
CN Acetamide, N-[2-[[2-[[4-(4-morpholinyl)phenyl]amino]-5-nitro-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

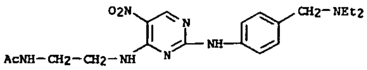


RN 514838-07-4 HCAPLUS
CN Methanesulfonamide, N-[4-[[4-[(trans-4-hydroxycyclohexyl)methylamino]-5-nitro-2-pyrimidinyl]amino]phenyl]-N-methyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.

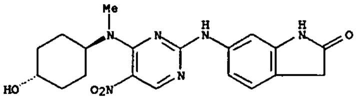


RN 514838-08-5 HCAPLUS
CN Acetamide, N-[2-[[2-[[4-[(diethylamino)methyl]phenyl]amino]-5-nitro-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

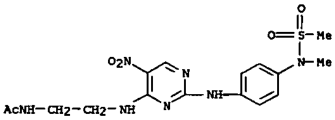


RN 514838-09-6 HCAPLUS
CN 2H-Indol-2-one, 1,3-dihydro-6-[[4-[(trans-4-hydroxycyclohexyl)methylamino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

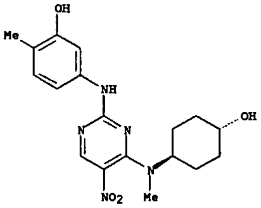


RN 514838-11-0 HCAPLUS
CN Acetamide, N-[2-[[2-[[4-[methyl(methylsulfonyl)amino]phenyl]amino]-5-nitro-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)



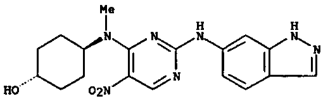
RN 514838-15-4 HCAPLUS
CN Phenol, 5-[[4-[(trans-4-hydroxycyclohexyl)methylamino]-5-nitro-2-pyrimidinyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.

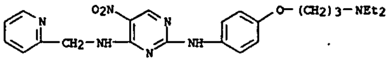


RN 514838-16-5 HCAPLUS
CN Cyclohexanol, 4-[[2-(1H-indazol-6-ylamino)-5-nitro-4-pyrimidinyl]methylamino]-, trans- (9CI) (CA INDEX NAME)

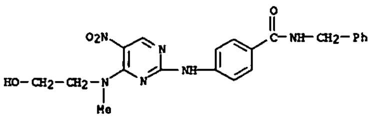
Relative stereochemistry.



RN 514838-18-7 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-[4-[3-(diethylamino)propoxy]phenyl]-5-nitro-N4-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)

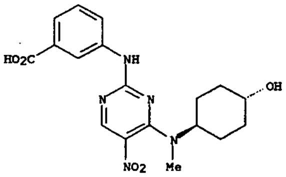


RN 514838-22-3 HCAPLUS
CN Benzamide, 4-[[4-[(2-hydroxyethyl)methylamino]-5-nitro-2-pyrimidinyl]amino]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

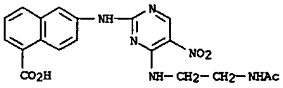


RN 514838-23-4 HCAPLUS
CN Benzoic acid, 3-[[4-[(trans-4-hydroxycyclohexyl)methylamino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

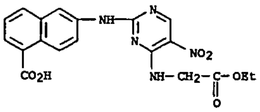
Relative stereochemistry.



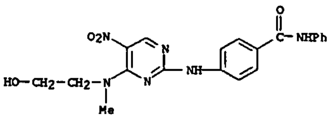
RN 514838-25-6 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 6-[[4-[[2-(acetylamino)ethyl]amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 514838-26-7 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 6-[[4-[(2-ethoxy-2-oxoethyl)amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 514838-27-8 HCAPLUS
CN Benzamide, 4-[[4-[(2-hydroxyethyl)methylamino]-5-nitro-2-pyrimidinyl]amino]-N-phenyl- (9CI) (CA INDEX NAME)

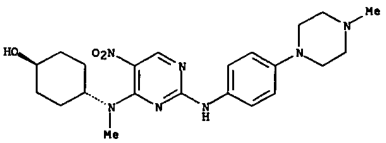


RN 514838-29-0 HCAPLUS

L4 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

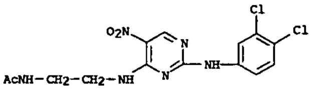
CN Cyclohexanol, 4-[methyl[2-[[4-(4-methyl-1-piperazinyl)phenyl]amino]-5-nitro-4-pyrimidinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 514843-25-5 HCAPLUS

CN Acetamide, N-[2-[[2-[(3,4-dichlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

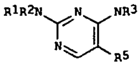


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 24 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 25 Apr 2003

GI



I

AB The title compds. [I; R1 = H, alkyl; R2 = (substituted) Ph; R3 = (substituted) alkyl, cycloalkyl, cycloalkylalkyl, arylalkyl, alkenyl, alkynyl; R4 = H, alkyl; or NR3R4 = (substituted) 3-7 membered alkylenimino; R5 = NO2, amino, alkylamino, dialkylamino, etc.], were prepared Thus, 2-chloro-4-methylamino-5-nitropyrimidine and 3,4-dichloroaniline were heated in the presence of sulfolane for 45 min at 160° in an oil bath to give 90% 2-(3,4-dichlorophenylamino)-4-methylamino-5-nitropyrimidine. Several I inhibited formation of β amyloid with IC50 = 4-1100 μM.

ACCESSION NUMBER: 2003:319718 HCAPLUS

DOCUMENT NUMBER: 138:338160

TITLE: Preparation of diaminopyrimidines as inhibitors of β amyloid formation or its release

INVENTOR(S): Himmelsbach, Frank; Fuchs, Klaus; Briem, Hans; Fechteler, Katja; Kostka, Markus; Dorner-Ciossek, Cornelia; Bornemann, Klaus; Klinder, Klaus

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany

SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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     PATENT NO.          KIND    DATE          APPLICATION NO.         DATE
     ---------------     ----    --------      --------------------    --------
     WO 2003032994        A2     20030424      WO 2002-EP11345         20021010
     WO 2003032994        A3     20030612
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
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     EP 1453516           A2     20040908      EP 2002-772368          20021010
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
     US 2003134838        A1     20030717      US 2002-272160          20021016
     US 2005090486        A1     20050428      US 2004-7923            20041209
PRIORITY APPLN. INFO.:                         US 2001-330128P      P  20011017
                                               WO 2002-EP11345      W  20021010
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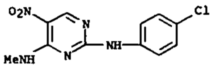
OTHER SOURCE(S): MARPAT 138:338160

L4 ANSWER 24 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT **515824-69-8P 515824-99-4P 515825-03-3P**
515825-21-5P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of diaminopyrimidines useful for inhibiting β amyloid formation or its release)

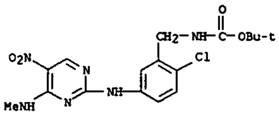
RN 515824-69-8 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



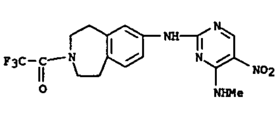
RN 515824-99-4 HCAPLUS

CN Carbamic acid, [[2-chloro-5-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



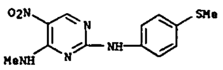
RN 515825-03-3 HCAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-N-[4-(methylamino)-5-nitro-2-pyrimidinyl]-3-(trifluoroacetyl)- (9CI) (CA INDEX NAME)



RN 515825-21-5 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-methyl-N2-[4-(methylthio)phenyl]-5-nitro- (9CI) (CA INDEX NAME)



IT **330550-94-2P 514831-70-0P 514832-07-6P**
514832-09-8P 514832-11-2P 514832-27-0P
514832-63-4P 514834-74-3P 514834-76-5P

L4 ANSWER 24 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

514834-78-7P 514834-99-2P 514835-13-3P
514835-15-5P 514835-19-9P 514835-60-0P
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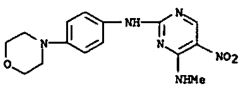
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of diaminopyrimidines useful for inhibiting β amyloid formation or its release)

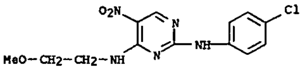
RN 330550-94-2 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-methyl-N2-[4-(4-morpholinyl)phenyl]-5-nitro- (9CI) (CA INDEX NAME)

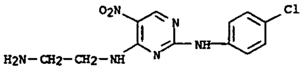


RN 514831-70-0 HCAPLUS

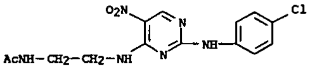
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-(2-methoxyethyl)-5-nitro- (9CI) (CA INDEX NAME)



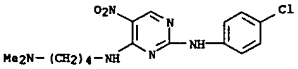
RN 514832-07-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-(2-aminoethyl)-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)



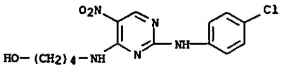
RN 514832-09-8 HCAPLUS
CN Acetamide, N-[2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)



RN 514832-11-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[4-(dimethylamino)butyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 514832-27-0 HCAPLUS
CN 1-Butanol, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 514832-63-4 HCAPLUS
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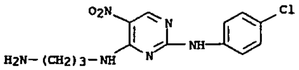

RN 514834-74-3 HCAPLUS
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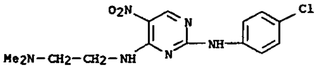

RN 514834-76-5 HCAPLUS
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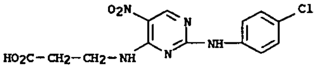

RN 514834-78-7 HCAPLUS
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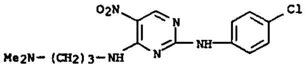
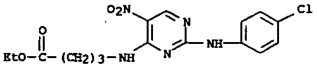
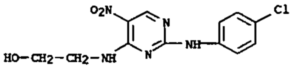


RN 514834-99-2 HCAPLUS
CN Butanoic acid, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

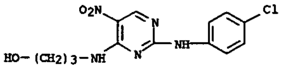


RN 514835-13-3 HCAPLUS

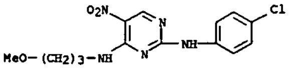
CN Ethanol, 2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



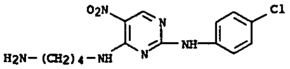
RN 514835-15-5 HCAPLUS
CN 1-Propanol, 3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 514835-19-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-(3-methoxypropyl)-5-nitro- (9CI) (CA INDEX NAME)



RN 514835-60-0 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-(4-aminobutyl)-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)



RN 514835-74-6 HCAPLUS
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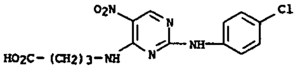
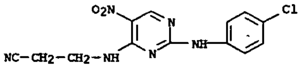
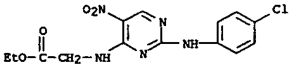


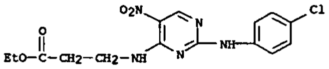
RN 514836-82-9 HCAPLUS
CN Propanenitrile, 3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



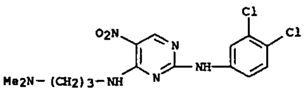
RN 514836-83-0 HCAPLUS
CN Glycine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)



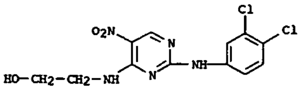
RN 514836-84-1 HCAPLUS
CN β-Alanine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)



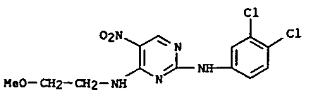
RN 514836-85-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-[3-(dimethylamino)propyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 514836-87-4 HCAPLUS
CN Ethanol, 2-[[2-[(3,4-dichlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 514836-89-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-(2-methoxyethyl)-5-nitro- (9CI) (CA INDEX NAME)



RN 514836-90-9 HCAPLUS
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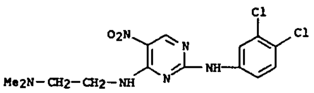

RN 514836-92-1 HCAPLUS
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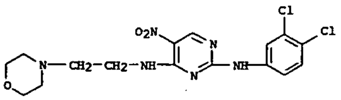
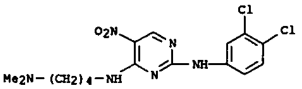
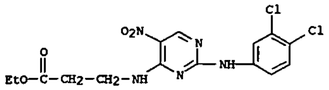


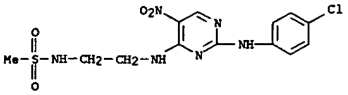
RN 514836-94-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-[4-(dimethylamino)butyl]-5-nitro- (9CI) (CA INDEX NAME)



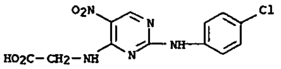
RN 514836-96-5 HCAPLUS
CN β-Alanine, N-[2-[(3,4-dichlorophenyl)amino]-5-nitro-4-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)



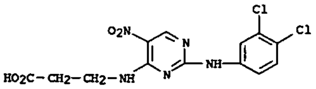
RN 514836-98-7 HCAPLUS
CN Methanesulfonamide, N-[2-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)



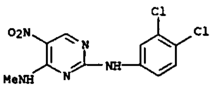
RN 514837-00-4 HCAPLUS
CN Glycine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



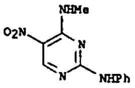
RN 514837-01-5 HCAPLUS
CN β-Alanine, N-[2-[(3,4-dichlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



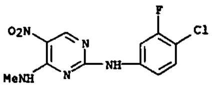
RN 515824-68-7 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



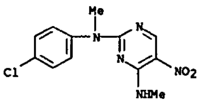
RN 515824-70-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-5-nitro-N2-phenyl- (9CI) (CA INDEX NAME)



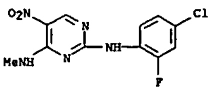
RN 515824-71-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chloro-3-fluorophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



RN 515824-72-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N2,N4-dimethyl-5-nitro- (9CI) (CA INDEX NAME)

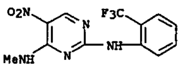


RN 515824-73-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chloro-2-fluorophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)

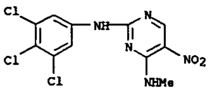


RN 515824-74-5 HCAPLUS

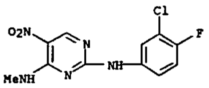
CN 2,4-Pyrimidinediamine, N4-methyl-5-nitro-N2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



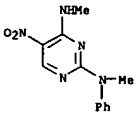
RN 515824-75-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-5-nitro-N2-(3,4,5-trichlorophenyl)- (9CI) (CA INDEX NAME)



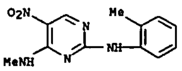
RN 515824-76-7 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3-chloro-4-fluorophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



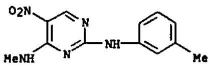
RN 515824-77-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N2,N4-dimethyl-5-nitro-N2-phenyl- (9CI) (CA INDEX NAME)



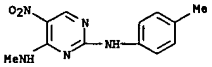
RN 515824-78-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-N2-(2-methylphenyl)-5-nitro- (9CI) (CA INDEX NAME)



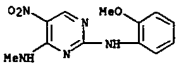
RN 515824-79-0 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-N2-(3-methylphenyl)-5-nitro- (9CI) (CA INDEX NAME)



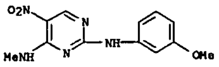
RN 515824-80-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-N2-(4-methylphenyl)-5-nitro- (9CI) (CA INDEX NAME)



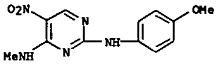
RN 515824-81-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(2-methoxyphenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



RN 515824-82-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3-methoxyphenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)

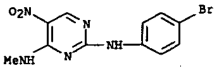


RN 515824-83-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-methoxyphenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)

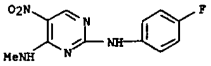


RN 515824-84-7 HCAPLUS

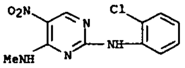
CN 2,4-Pyrimidinediamine, N2-(4-bromophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



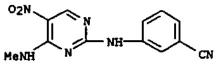
RN 515824-85-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-fluorophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



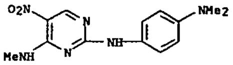
RN 515824-86-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(2-chlorophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



RN 515824-87-0 HCAPLUS
CN Benzonitrile, 3-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

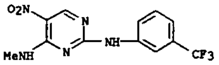


RN 515824-88-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-[4-(dimethylamino)phenyl]-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)

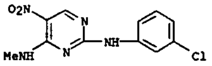


RN 515824-89-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-5-nitro-N2-[3-(trifluoromethyl)phenyl]-

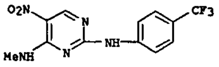
(9CI) (CA INDEX NAME)



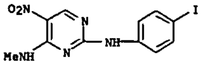
RN 515824-90-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



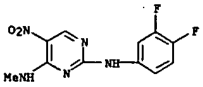
RN 515824-91-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-5-nitro-N2-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



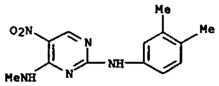
RN 515824-92-7 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-iodophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



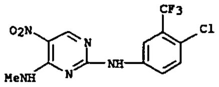
RN 515824-93-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-difluorophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



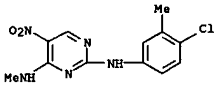
RN 515824-94-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dimethylphenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



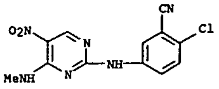
RN 515824-95-0 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-[4-chloro-3-(trifluoromethyl)phenyl]-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



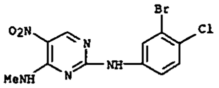
RN 515824-96-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chloro-3-methylphenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



RN 515824-97-2 HCAPLUS
CN Benzonitrile, 2-chloro-5-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

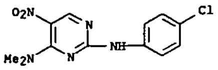


RN 515824-98-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3-bromo-4-chlorophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)

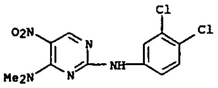


RN 515825-00-0 HCAPLUS

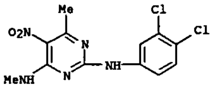
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4,N4-dimethyl-5-nitro- (9CI) (CA INDEX NAME)



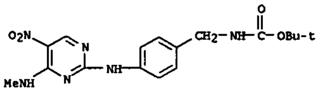
RN 515825-01-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4,N4-dimethyl-5-nitro- (9CI) (CA INDEX NAME)



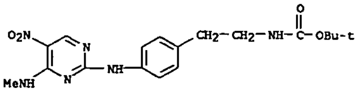
RN 515825-02-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4,6-dimethyl-5-nitro- (9CI) (CA INDEX NAME)



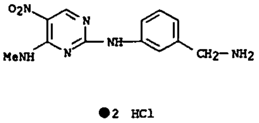
RN 515825-04-4 HCAPLUS
CN Carbamic acid, [[4-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



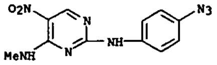
RN 515825-05-5 HCAPLUS
CN Carbamic acid, [2-[4-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]phenyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



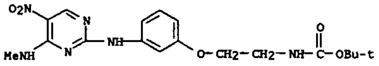
RN 515825-06-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-[3-(aminomethyl)phenyl]-N4-methyl-5-nitro-, dihydrochloride (9CI) (CA INDEX NAME)



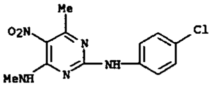
RN 515825-07-7 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-azidophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



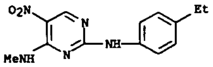
RN 515825-08-8 HCAPLUS
CN Carbamic acid, [2-[3-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]phenoxy]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



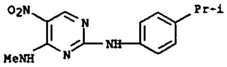
RN 515825-09-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4,6-dimethyl-5-nitro- (9CI) (CA INDEX NAME)



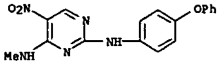
RN 515825-10-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-ethylphenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



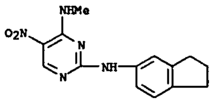
RN 515825-11-3 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-N2-[4-(1-methylethyl)phenyl]-5-nitro- (9CI) (CA INDEX NAME)



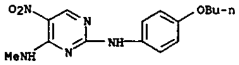
RN 515825-12-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-5-nitro-N2-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)



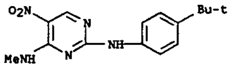
RN 515825-13-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(2,3-dihydro-1H-inden-5-yl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



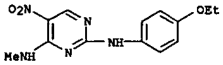
RN 515825-14-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-butoxyphenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



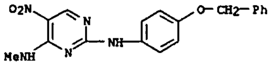
RN 515825-15-7 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-[4-(1,1-dimethylethyl)phenyl]-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



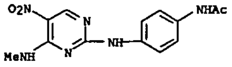
RN 515825-16-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-ethoxyphenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



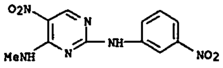
RN 515825-17-9 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-5-nitro-N2-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



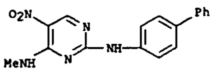
RN 515825-18-0 HCAPLUS
CN Acetamide, N-[4-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]phenyl]- (9CI) (CA INDEX NAME)



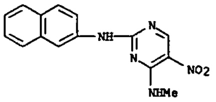
RN 515825-19-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-5-nitro-N2-(3-nitrophenyl)- (9CI) (CA INDEX NAME)



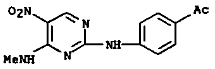
RN 515825-20-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-[1,1'-biphenyl]-4-yl-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



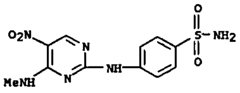
RN 515825-22-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-N2-2-naphthalenyl-5-nitro- (9CI) (CA INDEX NAME)



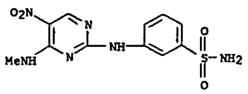
RN 515825-23-7 HCAPLUS
CN Ethanone, 1-[4-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]phenyl]- (9CI) (CA INDEX NAME)



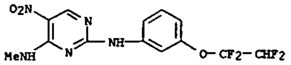
RN 515825-24-8 HCAPLUS
CN Benzenesulfonamide, 4-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



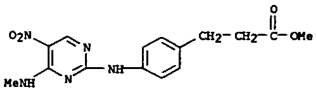
RN 515825-25-9 HCAPLUS
CN Benzenesulfonamide, 3-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



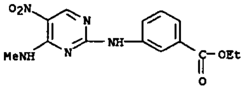
RN 515825-26-0 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-5-nitro-N2-[3-(1,1,2,2-tetrafluoroethoxy)phenyl]- (9CI) (CA INDEX NAME)



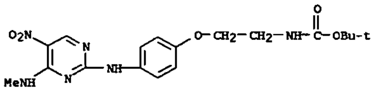
RN 515825-27-1 HCAPLUS
CN Benzenepropanoic acid, 4-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



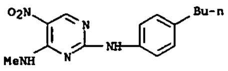
RN 515825-28-2 HCAPLUS
CN Benzoic acid, 3-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



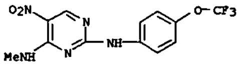
RN 515825-29-3 HCAPLUS
CN Carbamic acid, [2-[4-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]phenoxy]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



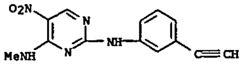
RN 515825-30-6 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-butylphenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



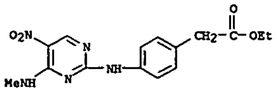
RN 515825-31-7 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-5-nitro-N2-[4-(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)



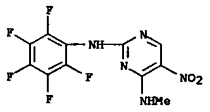
RN 515825-32-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3-ethynylphenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



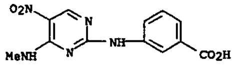
RN 515825-33-9 HCAPLUS
CN Benzeneacetic acid, 4-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



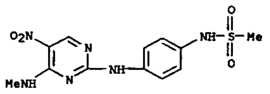
RN 515825-35-1 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-methyl-5-nitro-N2-(pentafluorophenyl)- (9CI) (CA INDEX NAME)



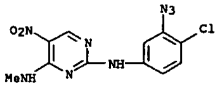
RN 515825-36-2 HCAPLUS
CN Benzoic acid, 3-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



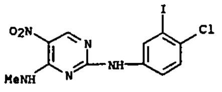
RN 515825-37-3 HCAPLUS
CN Methanesulfonamide, N-[4-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]phenyl]- (9CI) (CA INDEX NAME)



RN 515825-38-4 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(3-azido-4-chlorophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)

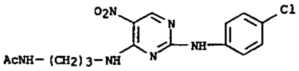


RN 515825-39-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chloro-3-iodophenyl)-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)



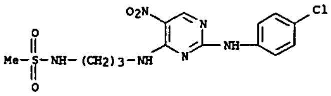
RN 515825-61-3 HCAPLUS

CN Acetamide, N-[3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]propyl]- (9CI) (CA INDEX NAME)



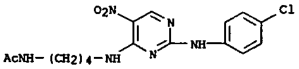
RN 515825-62-4 HCAPLUS

CN Methanesulfonamide, N-[3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]propyl]- (9CI) (CA INDEX NAME)



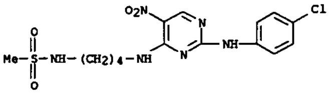
RN 515825-63-5 HCAPLUS

CN Acetamide, N-[4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]butyl]- (9CI) (CA INDEX NAME)



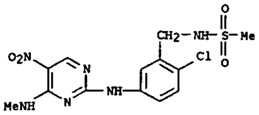
RN 515825-64-6 HCAPLUS

CN Methanesulfonamide, N-[4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]butyl]- (9CI) (CA INDEX NAME)



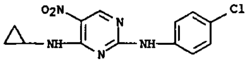
RN 515825-65-7 HCAPLUS

CN Methanesulfonamide, N-[[2-chloro-5-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]phenyl]methyl]- (9CI) (CA INDEX NAME)



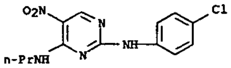
RN 515826-13-8 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-cyclopropyl-5-nitro- (9CI) (CA INDEX NAME)



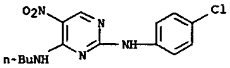
RN 515826-14-9 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-propyl- (9CI) (CA INDEX NAME)



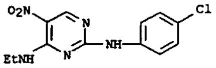
RN 515826-15-0 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-butyl-N2-(4-chlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)



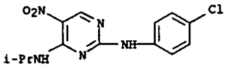
RN 515826-16-1 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-ethyl-5-nitro- (9CI) (CA INDEX NAME)



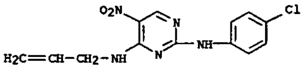
RN 515826-17-2 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-(1-methylethyl)-5-nitro- (9CI) (CA INDEX NAME)



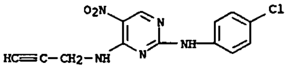
RN 515826-18-3 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-2-propenyl- (9CI) (CA INDEX NAME)



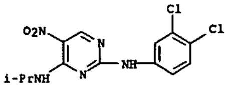
RN 515826-19-4 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-2-propynyl- (9CI) (CA INDEX NAME)



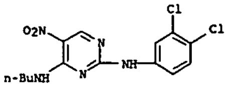
RN 515826-20-7 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-(1-methylethyl)-5-nitro- (9CI) (CA INDEX NAME)



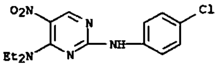
RN 515826-21-8 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-butyl-N2-(3,4-dichlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)



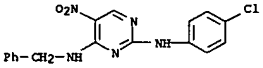
RN 515826-23-0 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4,N4-diethyl-5-nitro- (9CI) (CA INDEX NAME)



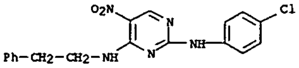
RN 515826-24-1 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-(phenylmethyl)- (9CI) (CA INDEX NAME)



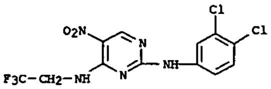
RN 515826-25-2 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-5-nitro-N4-(2-phenylethyl)- (9CI) (CA INDEX NAME)



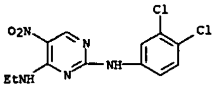
RN 515826-27-4 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-5-nitro-N4-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)



RN 515826-29-6 HCAPLUS

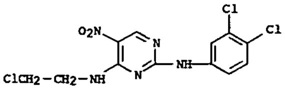
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-ethyl-5-nitro- (9CI) (CA INDEX NAME)



L4 ANSWER 24 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

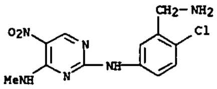
RN 515826-30-9 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-(2-chloroethyl)-N2-(3,4-dichlorophenyl)-5-nitro- (9CI) (CA INDEX NAME)



RN 515826-31-0 HCAPLUS

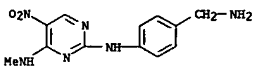
CN 2,4-Pyrimidinediamine, N2-[3-(aminomethyl)-4-chlorophenyl]-N4-methyl-5-nitro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 515826-32-1 HCAPLUS

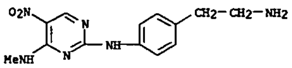
CN 2,4-Pyrimidinediamine, N2-[4-(aminomethyl)phenyl]-N4-methyl-5-nitro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 515826-33-2 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-[4-(2-aminoethyl)phenyl]-N4-methyl-5-nitro- (9CI) (CA INDEX NAME)

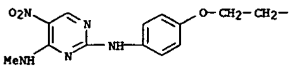


RN 515826-34-3 HCAPLUS

CN 2,4-Pyrimidinediamine, N2-[4-(2-aminoethoxy)phenyl]-N4-methyl-5-nitro-,

L4 ANSWER 24 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

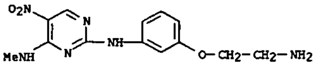
dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 515826-35-4 HCAPLUS

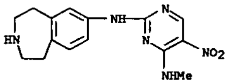
CN 2,4-Pyrimidinediamine, N2-[3-(2-aminoethoxy)phenyl]-N4-methyl-5-nitro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

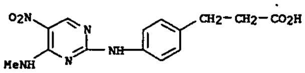
RN 515826-36-5 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-methyl-5-nitro-N2-(2,3,4,5-tetrahydro-1H-3-benzazepin-7-yl)- (9CI) (CA INDEX NAME)



RN 515826-37-6 HCAPLUS

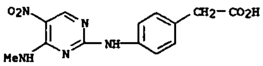
CN Benzenepropanoic acid, 4-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 515826-38-7 HCAPLUS

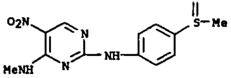
CN Benzeneacetic acid, 4-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

L4 ANSWER 24 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



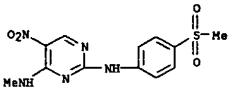
RN 515826-44-5 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-methyl-N2-[4-(methylsulfinyl)phenyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 515826-45-6 HCAPLUS

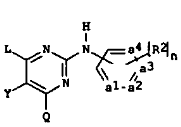
CN 2,4-Pyrimidinediamine, N4-methyl-N2-[4-(methylsulfonyl)phenyl]-5-nitro- (9CI) (CA INDEX NAME)



L4 ANSWER 25 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 16 Nov 2001

GI



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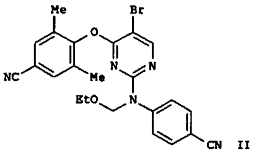

II

AB The title compds. A1A2NR1 [I; R1 = alkyl, SOR8, SO2R8, etc.; R8 = alkyl, (un)substituted Ph, (un)saturated heterocyclyl; A1A2N- is the covalently bonded form of the corresponding intermediate of the formula A1A2NH, which is a HIV replication inhibiting pyrimidine II (wherein a1:a2a3:a4 = CH:CHCH:CH, N:CHCH:CH, N:CHN:CH, N:CHCH:N, N:NCH:CH; n = 0-5; R2 = OH, halo, alkyl, etc.; L = alkyl, alkenyl, cycloalkyl, etc.; Q = H, alkyl, halo, etc.; Y = H, OH, halo, etc.)], were prepared Thus, reacting 4-({5-bromo-4-(4-cyano-2,6-dimethylphenoxy)-2-pyrimidinyl]amino)benzonitrile (preparation given) with (chloromethoxy)ethane in the presence of NaH in THF afforded 19% III. Anti-HIV activity of compds. I was tested and results were given.

ACCESSION NUMBER: 2001:833289 HCAPLUS
DOCUMENT NUMBER: 135:371756
TITLE: Preparation of prodrugs of HIV replication inhibiting pyrimidines
INVENTOR(S): Kukla, Michael Joseph; Ludovici, Donald William; Kavash, Robert W.; De Corte, Bart Lieven Daniel; Heeres, Jan; Janssen, Paul Adriaan Jan; Koymans, Lucien Maria Henricus; De Jonge, Marc Rene; Van Aken Koen, Jeanne Alfons; Krief, Alain
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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     PATENT NO.          KIND    DATE       APPLICATION NO.          DATE
     ---------------     ----  --------    --------------------    --------
     WO 2001085699        A2   20011115    WO 2001-EP4990          20010503
     WO 2001085699        A3   20020228
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM,
             HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,
             RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ,
             VN, YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     CA 2407754           AA   20011115    CA 2001-2407754         20010503
     AU 2001060277        A5   20011120    AU 2001-60277           20010503
     AU 782948            B2   20050915
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L4   ANSWER 25 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)
     EP 1282607            A2     20030212    EP 2001-933925          20010503
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2003532713         T2     20031105    JP 2001-582300          20010503
     US 2003186990         A1     20031002    US 2002-275333          20021107
     US 7034019            B2     20060425
     US 2006009474         A1     20060112    US 2005-225839          20050913
PRIORITY APPLN. INFO.:                        US 2000-202471P      P  20000508
                                              WO 2001-EP4990       W  20010503
                                              US 2002-275333       A3 20021107
OTHER SOURCE(S):          MARPAT 135:371756
IT   269055-21-2
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of prodrugs of HIV replication inhibiting pyrimidines)
RN   269055-21-2  HCAPLUS
CN   Benzonitrile, 4-[[5-nitro-4-[(2,4,6-trimethylphenyl)amino]-2-
     pyrimidinyl]amino]- (9CI)  (CA INDEX NAME)
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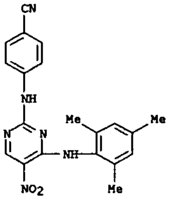

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L4   ANSWER 26 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  06 Apr 2001
GI
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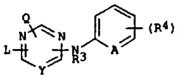

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AB   A particle consisting of a solid dispersion comprising ≥1
     pharmaceutically acceptable H2O-soluble polymers and a title compound, e.g.,
     [I; Y = CR5, N; A = CH, CR4, N; n = 0-4; Q = NR1R2, H; R1, R2 = H, OH,
     (substituted) alkyl, alkoxy, alkylcarbonyl, alkoxycarbonyl, aryl, etc.; or
     R1R2 = atoms to form pyrrolidinyl, piperidinyl, morpholinyl, azido,
     alkylaminoalkylidene; R3 = H, aryl, alkylcarbonyl, alkyl, alkoxycarbonyl,
     alkoxycarbonylalkyl; R4 = OH, halo, alkyl, alkoxy, cyano, aminocarbonyl,
     NO2, amino, trihalomethyl, trihalomethoxy, etc.; R5 = H, alkyl; L = X1R6,
     X2AR7, etc.; R6, R7 = (substituted) Ph, indanyl, indolyl; X1, X2 = NR3,
     NHNH, N:N, O, S, SO, SO2; A = C1-4 alkylene; with provisos], is claimed.
     Thus, 5-bromo-2-chloro-N-(2,4,6-trimethylphenyl)-4-pyrimidineamine (preparation
     given) was stirred with HCl in Et2O followed by evaporation of solvent, addition
     of 4-aminobenzonitrile and dioxane, and reflux for 4 days to give 2%
     4-[[5-chloro-2-[(2,4,6-trimethylphenyl)amino]-4-
     pyrimidinyl]amino]benzonitrile.  Tested title compds. showed anti-HIV
     activity with IC50 = 0.0004-0.030 µM.  A title compound melt extrudate
     was prepared using hydroxypropyl methylcellulose with no degradation of the
     active ingredient.
ACCESSION NUMBER:         2001:247156  HCAPLUS
DOCUMENT NUMBER:          134:280865
TITLE:                    Preparation of azinylaminobenzonitriles and related
                          compounds as virucides.
INVENTOR(S):              Verreck, Geert; Baert, Lieven
PATENT ASSIGNEE(S):       Janssen Pharmaceutica N.V., Belg.
SOURCE:                   PCT Int. Appl., 89 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   2
PATENT INFORMATION:

     PATENT NO.            KIND   DATE        APPLICATION NO.         DATE
     ---------------       ----   --------    --------------------    --------
     WO 2001022938          A1    20010405    WO 2000-EP8522          20000831
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     CA 2384188             AA    20010405    CA 2000-2384188         20000831
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L4   ANSWER 26 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)
     BR 2000014271         A      20020521    BR 2000-14271           20000831
     EP 1225874            A1     20020731    EP 2000-964080          20000831
     EP 1225874            B1     20060201
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL
     JP 2003510264         T2     20030318    JP 2001-526150          20000831
     EE 200200151          A      20030415    EE 2002-151             20000831
     NZ 517025             A      20030725    NZ 2000-517025          20000831
     TR 200200763          T2     20030922    TR 2002-200200763       20000831
     AU 775360             B2     20040729    AU 2000-75127           20000831
     AT 316781             E      20060215    AT 2000-964080          20000831
     BG 106521             A      20021229    BG 2002-106521          20020314
     ZA 2002002289         A      20030620    ZA 2002-2289            20020320
     NO 2002001443         A      20020322    NO 2002-1443            20020322
     AU 2004224973         A1     20041125    AU 2004-224973          20041029
PRIORITY APPLN. INFO.:                        EP 1999-203128       A  19990924
                                              WO 2000-EP8522       W  20000831
OTHER SOURCE(S):          MARPAT 134:280865
IT   269055-21-2P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
        (preparation of azinylaminobenzonitriles and related compds. as virucides)
RN   269055-21-2  HCAPLUS
CN   Benzonitrile, 4-[[5-nitro-4-[(2,4,6-trimethylphenyl)amino]-2-
     pyrimidinyl]amino]- (9CI)  (CA INDEX NAME)
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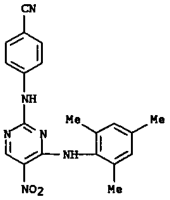

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IT   269055-10-9P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of azinylaminobenzonitriles and related compds. as virucides)
RN   269055-10-9  HCAPLUS
CN   Benzonitrile, 4-[[5-nitro-2-[(2,4,6-trimethylphenyl)amino]-4-
     pyrimidinyl]amino]- (9CI)  (CA INDEX NAME)
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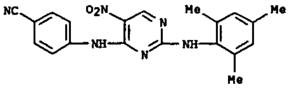

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L4   ANSWER 26 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)
REFERENCE COUNT:          5       THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
                                  RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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L4   ANSWER 27 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  22 Mar 2001
GI


* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

AB   The title compds. of formulas I, II, III and IV [W = NH, S, SO, SO2; R2 =
     (un)substituted aryl, heteroaryl, carbocycle, heterocycle; Q = H, alkyl;
     R4, R6, R9 = H, halogen, alkyl, alkoxy, (un)substituted aryl, heteroaryl,
     arylalkyl, heteroarylalkyl; R8 = H, alkyl, (un)substituted carbocycle,
     heterocycle, aryl etc.] and their pharmaceutically acceptable salts,
     inhibitors of cyclin-dependent kinase (cdks) and growth factor-mediated
     kinases, and useful for treating cell proliferative disorders, such as
     cancer and restenosis, were prepared  Thus, pteridinone derivative V was prepared
     by reaction of 5-amino-4-(methylamino)-2-[[4-(morpholin-4-
     yl)phenyl]amino]pyrimidine (also prepared) and Et 2-(2,6-dichlorophenyl)-2-
     oxoacetate, which showed IC50 of >7.7 µM against PDGF-receptor tyrosine
     kinase assay.  A method of treating cell proliferative disorders and
     pharmaceutical compns. were also claimed.
ACCESSION NUMBER:          2001:208274  HCAPLUS
DOCUMENT NUMBER:           134:237498
TITLE:                     Preparation of pteridinones as kinase inhibitors
INVENTOR(S):               Denny, Williams Alexander; Dobrusin, Ellen Myra;
                           Kramer, James Bernard; Mc Namara, Dennis Joseph;
                           Rewcastle, Gordon William; Showalter, Howard Daniel
                           Hollis; Toogood, Peter Laurence
PATENT ASSIGNEE(S):        Warner-Lambert Co., USA
SOURCE:                    PCT Int. Appl., 116 pp.
                           CODEN: PIXXD2
DOCUMENT TYPE:             Patent
LANGUAGE:                  English
FAMILY ACC. NUM. COUNT:    1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE       APPLICATION NO.          DATE
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     WO 2001019825        A1    20010322   WO 2000-US17037          20000621
         W:  AE, AG, AL, AU, BA, BB, BG, BR, BZ, CA, CN, CR, CU, CZ, DM, DZ,
             EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT,
             LV, MA, MG, MK, MN, MX, MZ, NO, NZ, PL, RO, SG, SI, SK, SL, TR,
             TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     CA 2393896           AA    20010322   CA 2000-2393896          20000621
     BR 2000013952        A     20020514   BR 2000-13952            20000621
     JP 2003509425        T2    20030311   JP 2001-523402           20000621
     EE 200200140         A     20030415   EE 2002-140              20000621
     NZ 516872            A     20031031   NZ 2000-516872           20000621
     EP 1409487           A1    20040421   EP 2000-941604           20000621
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, FI, CY
     AU 777468            B2    20041021   AU 2000-56295            20000621
     ZA 2002000896        A     20030430   ZA 2002-896              20020131
     US 2003130286        A1    20030710   US 2002-70530            20020306
     NO 2002001239        A     20020313   NO 2002-1239             20020313
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L4   ANSWER 27 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)
     BG 106594            A     20021229   BG 2002-106594           20020410
PRIORITY APPLN. INFO.:                     US 1999-154095P       P  19990915
                                           WO 2000-US17037       W  20000621
OTHER SOURCE(S):           MARPAT 134:237498
IT   330550-94-2P 330550-95-3P 330550-96-4P
     330550-97-5P 330550-98-6P 330551-00-3P
     330551-01-4P 330551-02-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of pteridinones for inhibiting kinase mediated cellular
        proliferative disorders)
RN   330550-94-2  HCAPLUS
CN   2,4-Pyrimidinediamine, N4-methyl-N2-[4-(4-morpholinyl)phenyl]-5-nitro-
     (9CI)  (CA INDEX NAME)
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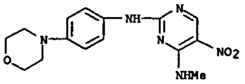

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RN   330550-95-3  HCAPLUS
CN   2,4-Pyrimidinediamine, N2-[4-[2-(diethylamino)ethoxy]phenyl]-N4-methyl-5-
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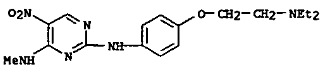

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RN   330550-96-4  HCAPLUS
CN   Benzamide, N,N-diethyl-4-[[4-(methylamino)-5-nitro-2-pyrimidinyl]amino]-
     (9CI)  (CA INDEX NAME)
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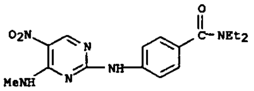

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RN   330550-97-5  HCAPLUS
CN   2,4-Pyrimidinediamine, N4-cyclopentyl-N2-[4-(4-morpholinyl)phenyl]-5-nitro-
     (9CI)  (CA INDEX NAME)
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L4   ANSWER 27 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)
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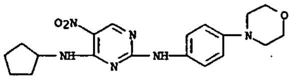

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RN   330550-98-6  HCAPLUS
CN   2,4-Pyrimidinediamine, N4-cyclopentyl-N2-[4-(4-methyl-1-
     piperazinyl)phenyl]-5-nitro- (9CI)  (CA INDEX NAME)
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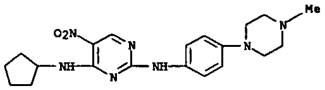

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RN   330551-00-3  HCAPLUS
CN   2,4-Pyrimidinediamine, N2-[4-[2-(diethylamino)ethoxy]phenyl]-N4-ethyl-5-
     nitro- (9CI)  (CA INDEX NAME)
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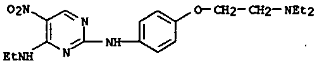

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RN   330551-01-4  HCAPLUS
CN   1-Piperazinecarboxylic acid, 4-[4-[[4-(cyclopentylamino)-5-nitro-2-
     pyrimidinyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI)  (CA INDEX NAME)
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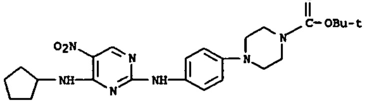

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RN   330551-02-5  HCAPLUS
CN   Carbamic acid, [1-[4-[[4-(cyclopentylamino)-5-nitro-2-
     pyrimidinyl]amino]phenyl]-3-pyrrolidinyl]-, 1,1-dimethylethyl ester (9CI)
     (CA INDEX NAME)
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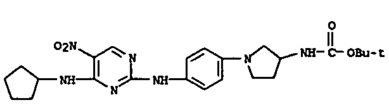

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L4   ANSWER 27 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN      (Continued)
IT   330551-21-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of pteridinones for inhibiting kinase mediated cellular
        proliferative disorders)
RN   330551-21-8  HCAPLUS
CN   2,4-Pyrimidinediamine, N4-cyclopentyl-N2-[4-[4-[4-(cyclopentylamino)-5-
     nitro-2-pyrimidinyl]-1-piperazinyl]phenyl]-5-nitro- (9CI)  (CA INDEX NAME)
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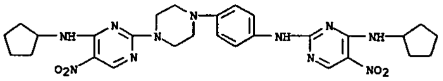

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REFERENCE COUNT:         5       THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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L4   ANSWER 28 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  07 Jul 2000
GI
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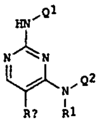

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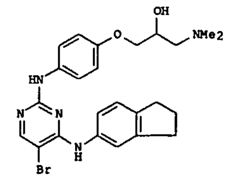

II

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AB   The present invention relates to the title compds. (I) [wherein R1 = H,
     (un)substituted alkyl, alkenyl, or alkynyl, benzyl, 2-phenylethyl,
     phthalimidoalkyl, or cycloalkylalkyl; Rx = halo, OH, NO2, NH2, CN, SH,
     CO2H, SO2NH2, NHCHO, ureido, etc.; Q1 and Q2 = independently
     (un)substituted aryl, 5- or 6-membered monocycle, or 9- or 10-membered
     bicyclic heterocycle], processes for their manufacture, and pharmaceutical
     compns. containing them.  For example, addition of 4-[2-hydroxy-3-(N,N-
     dimethylamino)propoxy]aniline•HCl in MeOH to 5-bromo-2-chloro-4-(indan-
     5-ylamino)pyrimidine in BuOH (prepns. given) and heating to 100°C
     for 18 h gave II (42%).  I inhibited the effects of cylin-dependent
     serine/threonine kinases (CDKs), showing selectivity for CDK2 (no data),
     CDK4 (IC50 ranging from 0.02 μM to 0.07 μM), and CDK6 (no data).  In
     a tyrosine kinase activity assay using Sf21 cells transfected with
     plaque-pure FAK recombinant virus, I also inhibited focal adhesion kinase
     3 (FAK3) with IC50 ranging from 0.032 μM to 0.07 μM.  Typical IC50
     values for I when tested for inhibition of cell growth in an
     Sulforhodamine B (SRB) assay were in the range of 1 mM to 1 nM.  Thus, I
     possess anti-cancer properties, including anti-cell-migration,
     antiproliferation and/or apoptotic properties.  Such properties are
     expected to be of value in the treatment of disease states associated with
     aberrant cell cycles and cell proliferation such as cancers (solid tumors
     and leukemias), fibroproliferative and differentiative disorders,
     psoriasis, rheumatoid arthritis, Kaposi's sarcoma, hemangioma, acute and
     chronic nephropathies, atheroma, atherosclerosis, arterial restenosis,
     autoimmune diseases, acute and chronic inflammation, bone diseases, and
     ocular diseases with retinal vessel proliferation.
ACCESSION NUMBER:         2000:457043  HCAPLUS
DOCUMENT NUMBER:          133:89537
TITLE:                    Preparation of 2,4-pyrimidinediamine derivatives as
                          anticancer agents
INVENTOR(S):              Bradbury, Robert Hugh; Breault, Gloria Anne; Jewsbury,
                          Philip John; Pease, Janet Elizabeth
PATENT ASSIGNEE(S):       Astrazeneca UK Limited, UK
SOURCE:                   PCT Int. Appl., 137 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
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L4   ANSWER 28 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE          APPLICATION NO.        DATE
     ---------------     ----   --------      --------------------   --------
     WO 2000039101        A1    20000706      WO 1999-GB4325         19991220
         W:  AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
             CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
             MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
             SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     CA 2352896           AA    20000706      CA 1999-2352896        19991220
     EP 1140860           A1    20011010      EP 1999-962375         19991220
     EP 1140860           B1    20040922
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     BR 9916590           A     20011023      BR 1999-16590          19991220
     JP 2002533446        T2    20021008      JP 2000-591012         19991220
     AU 763091            B2    20030710      AU 2000-18743          19991220
     NZ 512118            A     20030829      NZ 1999-512118         19991220
     AT 277020            E     20041015      AT 1999-962375         19991220
     PT 1140860           T     20050131      PT 1999-962375         19991220
     ES 2228145           T3    20050401      ES 1999-962375         19991220
     ZA 2001004413        A     20020829      ZA 2001-4413           20010529
     NO 2001003038        A     20010822      NO 2001-3038           20010619
     NO 319815            B1    20050919
     US 6593326           B1    20030715      US 2001-868602         20010823
PRIORITY APPLN. INFO.:                        GB 1998-28511       A  19981224
                                              WO 1999-GB4325      W  19991220
OTHER SOURCE(S):         MARPAT 133:89537
IT   280579-00-2P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
        (preparation of 2,4-pyrimidinediamine anticancer agents by coupling
        halopyrimidines with anilines and optional derivatization)
RN   280579-00-2  HCAPLUS
CN   2-Propanol, 1-(dimethylamino)-3-[4-[[5-nitro-4-(phenylamino)-2-
     pyrimidinyl]amino]phenoxy]- (9CI)  (CA INDEX NAME)
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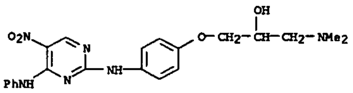

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IT   280578-86-1P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of 2,4-pyrimidinediamine anticancer agents by coupling
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L4   ANSWER 28 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
        halopyrimidines with anilines and optional derivatization)
RN   280578-86-1  HCAPLUS
CN   2-Propanol, 1-(dimethylamino)-3-[4-[[4-[(2-fluorophenyl)amino]-5-nitro-2-
     pyrimidinyl]amino]phenoxy]- (9CI)  (CA INDEX NAME)
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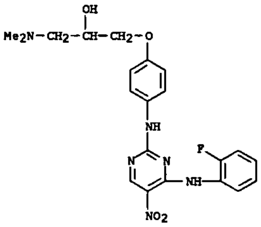

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REFERENCE COUNT:          4         THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
                                    RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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L4   ANSWER 29 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  19 May 2000
GI
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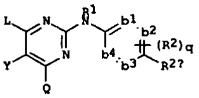

I

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AB   Title compds. [I; b1:b2CR2a:b3b4 = CH:CHCR2a:CHCH, N:CHCR2a:CHCH,
     CH:NCR2a:CHCH, N:NCR2a:CHCH, CH:NCR2a:NCH, etc.; q = 0-4; R1 = H, aryl,
     CHO, formylalkyl, alkylcarbonyl alkyl, alkoxycarbonyl, etc.; R2a = cyano,
     aminocarbonyl, cyanoalkyl, cyanoalkenyl, cyanoalkynyl, etc.; R2 = OH,
     halo, (substituted) alkyl, cycloalkyl, alkenyl, alkynyl, alkoxy, etc.; L =
     (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, XR3; R3 = (substituted)
     Ph, pyridyl, pyrimidnyl, pyrazinyl, pyridazinyl; X = NR1, NHNH, N:N, O,
     CO, S, SO, SO2, CHOH; Q = H, alkyl, halo, polyhaloalkyl, amino; Y = OH,
     halo, cycloalkyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl, substituted
     alkyl, etc.], were prepared  Thus, 5-bromo-4-chloro-N-(2,4,6-
     trimethylphenyl)-2-pyrimidineamine (preparation given) was treated with HCl in
     Et2O followed by solvent evaporation; 4-aminobenzonitrile and 1,4-dioxane were
     added and the mixture was refluxed 4 days to give 4-[[5-chloro-2-[(2,4,6-
     trimethylphenyl)amino]-4-pyrimidinyl]amino]benzonitrile.  The latter
     inhibited HIV-1 infection of MT-4 cells with IC50 = 0.004 μM.
ACCESSION NUMBER:         2000:335393  HCAPLUS
DOCUMENT NUMBER:          132:347578
TITLE:                    Preparation of arylaminopyrimidines as inhibitors of
                          HIV replication.
INVENTOR(S):              De Corte, Bart; De Jonge, Marc Rene; Heeres, Jan; Ho,
                          Chih Yung; Janssen, Paul Adriaan Jan; Kavash, Robert
                          W.; Koymans, Lucien Maria Henricus; Kukla, Michael
                          Joseph; Ludovici, Donald William; Van Aken, Koen
                          Jeanne Alfons
PATENT ASSIGNEE(S):       Janssen Pharmaceutica N.V., Belg.; et al.
SOURCE:                   PCT Int. Appl., 49 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE          APPLICATION NO.        DATE
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     WO 2000027825        A1    20000518      WO 1999-EP7417         19990924
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             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD,
             MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK,
             SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     CA 2350801           AA    20000518      CA 1999-2350801        19990924
     AU 9962008           A1    20000529      AU 1999-62008          19990924
     AU 762523            B2    20030626
     BR 9915552           A     20010814      BR 1999-15552          19990924
     TR 200101306         T2    20011022      TR 2001-200101306      19990924
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L4   ANSWER 29 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
     JP 2002529456          T2     20020910    JP 2000-581005          19990924
     EE 200100252           A      20021015    EE 2001-252             19990924
     NZ 511116              A      20030829    NZ 1999-511116          19990924
     EP 1002795             A1     20000524    EP 1999-203590          19991101
     EP 1002795             B1     20030305
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     EP 1270560             A1     20030102    EP 2002-18455           19991101
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL
     AT 233740              E      20030315    AT 1999-203590          19991101
     US 2003114472          A1     20030619    US 1999-430966          19991101
     US 6878717             B2     20050412
     PT 1002795             T      20030731    PT 1999-203590          19991101
     ES 2193664             T3     20031101    ES 1999-203590          19991101
     HK 1025330             A1     20030613    HK 2000-104633          20000726
     HR 2001000161          A1     20020228    HR 2001-161             20010307
     NO 2001001696          A      20010404    NO 2001-1696            20010404
     NO 318801              B1     20050509
     BG 105418              A      20011130    BG 2001-105418          20010406
     ZA 2001003769          A      20020812    ZA 2001-3769            20010509
     US 2004039005          A1     20040226    US 2003-634682          20030805
     US 7037917             B2     20060502
     US 2005288278          A1     20051229    US 2005-204513          20050816
PRIORITY APPLN. INFO.:                         US 1998-107792P      P  19981110
                                               US 1999-143962P      P  19990715
                                               US 1998-107792       P  19981110
                                               US 1999-143962       P  19990715
                                               WO 1999-EP7417       W  19990924
                                               EP 1999-203590       A3 19991101
                                               US 1999-430966       A1 19991101
                                               US 2003-634682       A1 20030805
OTHER SOURCE(S):          MARPAT 132:347578
IT   269055-10-9P 269055-21-2P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of arylaminopyrimidines as inhibitors of HIV replication)
RN   269055-10-9  HCAPLUS
CN   Benzonitrile, 4-[[5-nitro-2-[(2,4,6-trimethylphenyl)amino]-4-
     pyrimidinyl]amino]- (9CI)  (CA INDEX NAME)
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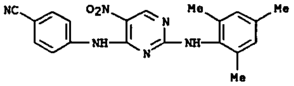

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RN   269055-21-2  HCAPLUS
CN   Benzonitrile, 4-[[5-nitro-4-[(2,4,6-trimethylphenyl)amino]-2-
     pyrimidinyl]amino]- (9CI)  (CA INDEX NAME)
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L4   ANSWER 29 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
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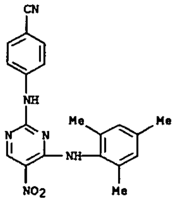

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REFERENCE COUNT:          1      THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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L4   ANSWER 30 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  06 Apr 1991
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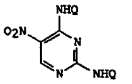

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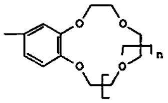

Q

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AB   Title compds. I (n = 1, 2, 3) were prepared by condensation of
     2,4-dichloro-5-nitropyrimidine with QNH2.  I (n = 1, 2) showed high
     extractive power for sodium and potassium resp.
ACCESSION NUMBER:         1991:122326  HCAPLUS
DOCUMENT NUMBER:          114:122326
TITLE:                    Bis-crown ethers containing pyrimidine ring. (I)
AUTHOR(S):                Lu, Guoyuan; Wang, Defeng; Hu, Houngweng
CORPORATE SOURCE:         Dep. Chem., Nanjing Univ., Nanjing, Peop. Rep. China
SOURCE:                   Nanjing Daxue Xuebao, Ziran Kexue (1990), 26(2),
                          348-51
                          CODEN: NCHPAZ; ISSN: 0469-5097
DOCUMENT TYPE:            Journal
LANGUAGE:                 Chinese
OTHER SOURCE(S):          CASREACT 114:122326
IT   124727-82-8P 124727-85-1P 124727-88-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation and extraction by, of alkali metals)
RN   124727-82-8  HCAPLUS
CN   2,4-Pyrimidinediamine, N,N'-bis(2,3,5,6,8,9-hexahydro-1,4,7,10-
     benzotetraoxacyclododecin-12-yl)-5-nitro- (9CI)  (CA INDEX NAME)
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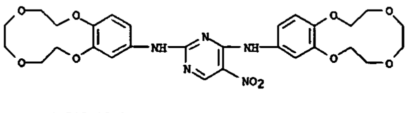

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RN   124727-85-1  HCAPLUS
CN   2,4-Pyrimidinediamine, 5-nitro-N,N'-bis(2,3,5,6,8,9,11,12-octahydro-
     1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)- (9CI)  (CA INDEX NAME)
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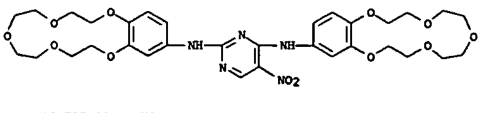

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RN   124727-88-4  HCAPLUS
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L4   ANSWER 30 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN     (Continued)
CN   2,4-Pyrimidinediamine, N,N'-bis(2,3,5,6,8,9,11,12,14,15-decahydro-
     1,4,7,10,13,16-benzohexaoxacyclooctadecin-18-yl)-5-nitro- (9CI)  (CA INDEX
     NAME)
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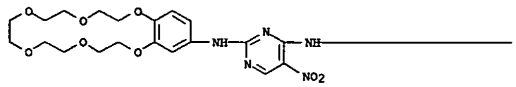
PAGE 1-A



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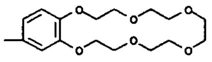
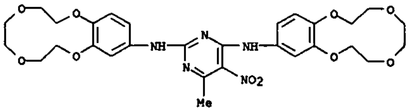
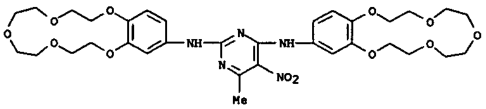


L4 ANSWER 31 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 26 May 1990
AB Six bis-crown ethers containing benzo-12-crown-4, benzo-15-crown-5 and benzo-18-crown-6 moieties bridged by a pyrimidine ring were prepared by the reaction of 4,6-dichloro-5-nitropyrimidine or 2,4-dichloro-5-nitro-6-methylpyrimidine with the 4'-aminobenzocrown ethers, resp. Extns. were carried out with aqueous solns. of alkali metal picrates with these bis-crown ether solns. in CHCl3. The extraction equilibrium consts. were also evaluated. The
title compound are effective extracting reagents for Na, K, and Cs, resp. The cation-selectivity is more effective than the corresponding monocyclic crown ethers.
ACCESSION NUMBER: 1990:198343 HCAPLUS
DOCUMENT NUMBER: 112:198343
TITLE: Bis-crown ether containing pyrimidine ring. (II)
AUTHOR(S): Lu, Guoyuan; Wang, Defen; Hu, Hongwen
CORPORATE SOURCE: Dep. Chem., Nanjing Univ., Nanjing, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1989), 10(8), 812-16
CODEN: KTHPDM; ISSN: 0251-0790
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
IT **124727-84-0P 124727-87-3P 124727-90-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interaction by, of alkali metals)
RN 124727-84-0 HCAPLUS
CN 2,4-Pyrimidinediamine, N,N'-bis(2,3,5,6,8,9-hexahydro-1,4,7,10-benzotetraoxacyclododecin-12-yl)-6-methyl-5-nitro- (9CI) (CA INDEX NAME)

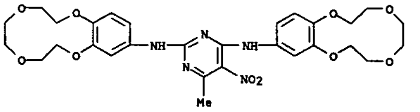


RN 124727-87-3 HCAPLUS
CN 2,4-Pyrimidinediamine, 6-methyl-5-nitro-N,N'-bis(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)- (9CI) (CA INDEX NAME)



RN 124727-90-8 HCAPLUS
CN 2,4-Pyrimidinediamine, N,N'-bis(2,3,5,6,8,9,11,12,14,15-decahydro-1,4,7,10,13,16-benzohexaoxacyclooctadecin-18-yl)-6-methyl-5-nitro- (9CI) (CA INDEX NAME)

L4 ANSWER 32 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1990
AB The characteristics of eight crown ether stationary phases in gas chromatog. are discussed through the determination of the McReynolds consts. These crowns ether stationary phases were compared with OV-17, OV-225, and PEG-600 based on the McReynolds consts. The reason for having different McReynolds consts. for the crown ethers is attributed to the differences of their structures. Special uses for some crown ethers are introduced. The accuracies of the consts. were examined
ACCESSION NUMBER: 1990:191083 HCAPLUS
DOCUMENT NUMBER: 112:191083
TITLE: Study on McReynolds constants of eight crown ether stationary phases
AUTHOR(S): Shi, Jian; Lu, Guoyuan; Guo, Wei; Wang, Defen; Hu, Hongwen
CORPORATE SOURCE: Dep. Chem., Nanjing Univ., Nanjing, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1989), 10(6), 647-9
CODEN: KTHPDM; ISSN: 0251-0790
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
IT **124727-84-0**
RL: ANST (Analytical study)
(as stationary phase in gas chromatog., McReynolds consts. of)
RN 124727-84-0 HCAPLUS
CN 2,4-Pyrimidinediamine, N,N'-bis(2,3,5,6,8,9-hexahydro-1,4,7,10-benzotetraoxacyclododecin-12-yl)-6-methyl-5-nitro- (9CI) (CA INDEX NAME)



L4 ANSWER 31 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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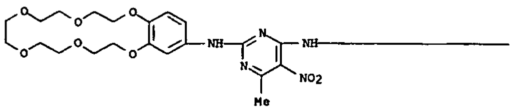
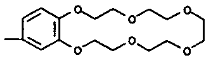
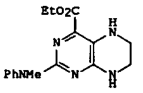


PAGE 1-B

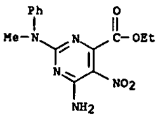


L4 ANSWER 33 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 17 Feb 1990
GI

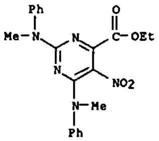


I

AB In the search for a model tetrahydropteridine which would be stable in air and soluble in organic solvents, the title compound (I) was prepared which was found
to fit both of these criteria. In the course of the synthesis, a series of new pyrimidine derivs. was prepared and characterized.
ACCESSION NUMBER: 1990:55445 HCAPLUS
DOCUMENT NUMBER: 112:55445
TITLE: New derivatives of 5-nitroorotic acid, and the synthesis of 4-ethoxycarbonyl-2-(N-methylanilino)-5,6,7,8-tetrahydropteridine
AUTHOR(S): Boyle, Peter H.; Gillespie, Paul
CORPORATE SOURCE: Univ. Chem. Lab., Trinity Coll., Dublin, Ire.
SOURCE: Journal of Chemical Research, Synopses (1989), (9), 282
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:55445
IT **124764-20-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 124764-20-1 HCAPLUS
CN 4-Pyrimidinecarboxylic acid, 6-amino-2-(methylphenylamino)-5-nitro-, ethyl ester (9CI) (CA INDEX NAME)



IT **124764-16-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 124764-16-5 HCAPLUS
CN 4-Pyrimidinecarboxylic acid, 2,6-bis(methylphenylamino)-5-nitro-, ethyl ester (9CI) (CA INDEX NAME)



ED Entered STN: 04 Feb 1990

AB Sodium-, potassium-, and cesium-ion-selective PVC membrane electrodes based on nine new bis-crown ethers containing benzo-12-crown-4, benzo-15-crown-5, and benzo-18-crown-6 moieties bridged by pyrimidine ring were prepared and their electrode behaviors were evaluated. The electrodes exhibited high selectivities for sodium, potassium, and cesium.

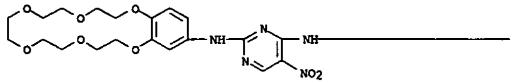
ACCESSION NUMBER:	1990:47701 HCAPLUS
DOCUMENT NUMBER:	112:47701
TITLE:	Bis-crown ether containing pyrimidine ring. III. Sodium, potassium and cesium ion selective PVC membrane electrodes based on bis-crown ethers as carrier
AUTHOR(S):	Lu, Guoyuan; Wang, Denfeng; Hu, Hungweng
CORPORATE SOURCE:	Dep. Chem., Nanjing Univ., Nanjing, Peop. Rep. China
SOURCE:	Wuji Huaxue (1988), 4(4), 91-6 CODEN: WUHUE7
DOCUMENT TYPE:	Journal
LANGUAGE:	Chinese

IT **124727-88-4 124727-90-8**
RL: ANST (Analytical study)
(cesium-selective membrane electrode based on)

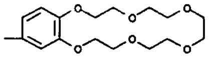
RN 124727-88-4 HCAPLUS

CN 2,4-Pyrimidinediamine, N,N'-bis(2,3,5,6,8,9,11,12,14,15-decahydro-1,4,7,10,13,16-benzohexaoxacyclooctadecin-18-yl)-5-nitro- (9CI) (CA INDEX NAME)

PAGE 1-A



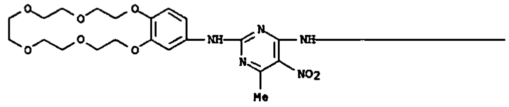
PAGE 1-B



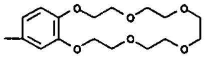
RN 124727-90-8 HCAPLUS

CN 2,4-Pyrimidinediamine, N,N'-bis(2,3,5,6,8,9,11,12,14,15-decahydro-1,4,7,10,13,16-benzohexaoxacyclooctadecin-18-yl)-6-methyl-5-nitro- (9CI) (CA INDEX NAME)

PAGE 1-A



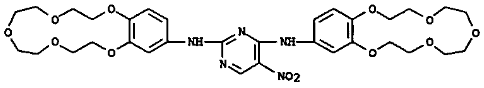
PAGE 1-B



IT **124727-85-1 124727-87-3**
RL: ANST (Analytical study)
(potassium-selective membrane electrode base on)

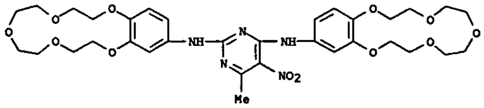
RN 124727-85-1 HCAPLUS

CN 2,4-Pyrimidinediamine, 5-nitro-N,N'-bis(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)- (9CI) (CA INDEX NAME)



RN 124727-87-3 HCAPLUS

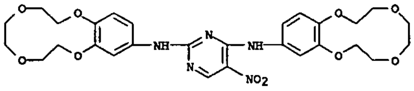
CN 2,4-Pyrimidinediamine, 6-methyl-5-nitro-N,N'-bis(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)- (9CI) (CA INDEX NAME)



IT **124727-82-8 124727-84-0**
RL: ANST (Analytical study)
(sodium-selective membrane electrode based on)

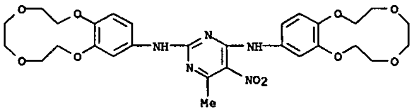
RN 124727-82-8 HCAPLUS

CN 2,4-Pyrimidinediamine, N,N'-bis(2,3,5,6,8,9-hexahydro-1,4,7,10-benzotetraoxacyclododecin-12-yl)-5-nitro- (9CI) (CA INDEX NAME)

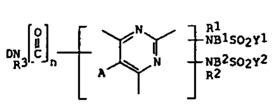


RN 124727-84-0 HCAPLUS

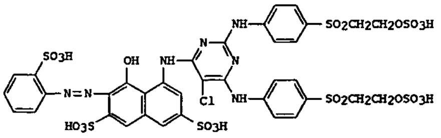
CN 2,4-Pyrimidinediamine, N,N'-bis(2,3,5,6,8,9-hexahydro-1,4,7,10-benzotetraoxacyclododecin-12-yl)-6-methyl-5-nitro- (9CI) (CA INDEX NAME)



L4 ANSWER 35 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 03 Apr 1989
GI



I



II

AB The title reactive dyes I [D = dye residue; n = 0.1; A = H, Cl, Br, Me, NO2, CN, carboxy, sulfo; R1-R3 = H, (un)substituted alkyl; B1, B2 = (un)substituted phenylene, naphthylene; Y1, Y2 = CH2CH2L, vinyl; L = alkali-removable group], useful for dyeing and printing cotton, are prepared. 2,4,6-Trifluoro-5-chloropyrimidine was condensed with 1-amino-8-hydroxy-7-(o-sulfophenylazo)-3,6-naphthalenedisulfonic acid, p-H2NC6H4SO2CH2CH2OSO3H, and m-H2NC6H4SO2CH2CH2OSO3H, and salted to give II (Na salt), λmax 540 nm (fabric color not specified).

ACCESSION NUMBER: 1989:116656 HCAPLUS
DOCUMENT NUMBER: 110:116656
TITLE: Pyrimidine compounds for dyeing and printing fiber materials
INVENTOR(S): Morimitsu, Toshihiko; Omura, Takashi
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63207860	A2	19880829	JP 1987-42224	19870224
JP 08026237	B4	19960313		

PRIORITY APPLN. INFO.: JP 1987-42224 19870224
OTHER SOURCE(S): MARPAT 110:116656

IT **118521-57-6P**
RL: IMF (Industrial manufacture); RCT (Reactant); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(manufacture of, as reactive dye for cotton)
RN 118521-57-6 HCAPLUS

L4 ANSWER 35 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,7-Naphthalenedisulfonic acid, 5-(benzoylamino)-4-hydroxy-3-[[5-[[2-[[2-methoxy-5-methyl-4-[[2-(sulfooxy)ethyl]sulfonyl]phenyl]amino]-5-nitro-6-[[3-[[2-(sulfooxy)ethyl]sulfonyl]phenyl]amino]-4-pyrimidinyl]amino]-2,4-disulfophenyl]azo]- (9CI) (CA INDEX NAME)

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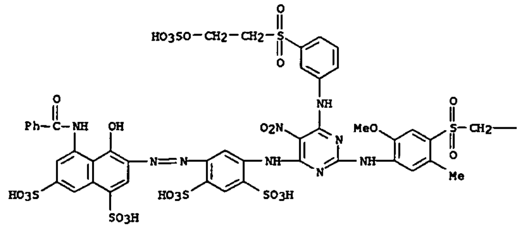
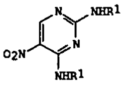


PAGE 1-B

—CH2—OSO3H

L4 ANSWER 36 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 Nov 1988
GI

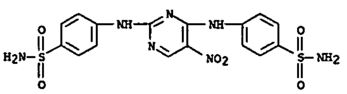


I

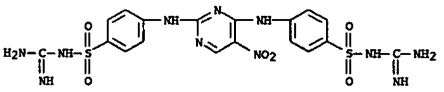
AB 2,4-Dichloro-5-nitropyrimidine was treated with amines to give pyrimidinediamines I [R1 = H2NSO2C6H4, substituted sulfamoylphenyl, HO(EtO2C)C6H3, H2NC6H4, HOC6H4, Cl(HO)C6H3, CH2CH2NH2, furfuryl, antipyrinyl, substituted pyrimidinyl]. Also prepared, from I (R1 = NH2), were I (R1 = NHCO2Et) and I (R1 = N:CHC6H4NO2-4).

ACCESSION NUMBER: 1988:570352 HCAPLUS
DOCUMENT NUMBER: 109:170352
TITLE: 2,4-bis(substituted) 5-nitropyrimidines of expected diuretic action
AUTHOR(S): El-Kerdawy, M. M.; Zayed, A. A.; Abou Hamid, M. M.
CORPORATE SOURCE: Natl. Org. Drug Control Res., Cairo, Egypt
SOURCE: Egyptian Journal of Chemistry (1987), Volume Date 1986, 29(2), 247-51
CODEN: EGJCA3; ISSN: 0367-0422
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **116859-92-8P 116859-93-9P 116859-94-0P**
116859-95-1P 116859-96-2P 116859-97-3P
116859-98-4P 116859-99-5P 116860-00-5P
116860-01-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 116859-92-8 HCAPLUS
CN Benzenesulfonamide, 4,4'-[(5-nitro-2,4-pyrimidinediyl)diimino]bis- (9CI) (CA INDEX NAME)

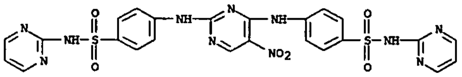


RN 116859-93-9 HCAPLUS
CN Benzenesulfonamide, 4,4'-[(5-nitro-2,4-pyrimidinediyl)diimino]bis[N-(aminoiminomethyl)- (9CI) (CA INDEX NAME)



RN 116859-94-0 HCAPLUS

L4 ANSWER 36 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzenesulfonamide, 4,4'-[(5-nitro-2,4-pyrimidinediyl)diimino]bis[N-2-pyrimidinyl- (9CI) (CA INDEX NAME)



RN 116859-95-1 HCAPLUS
CN Benzenesulfonamide, 4,4'-[(5-nitro-2,4-pyrimidinediyl)diimino]bis[N-(4-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

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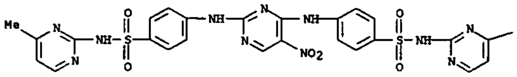

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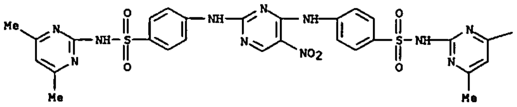
—Me

RN 116859-96-2 HCAPLUS
CN Benzenesulfonamide, 4,4'-[(5-nitro-2,4-pyrimidinediyl)diimino]bis[N-(4,6-dimethyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

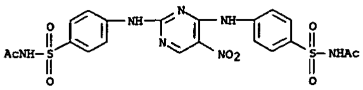


PAGE 1-B

—Me

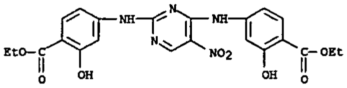
RN 116859-97-3 HCAPLUS
CN Acetamide, N,N'-[(5-nitro-2,4-pyrimidinediyl)bis(imino-4,1-phenylenesulfonyl)]bis- (9CI) (CA INDEX NAME)

L4 ANSWER 36 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



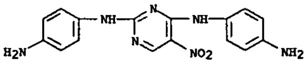
RN 116859-98-4 HCAPLUS

CN Benzoic acid, 4,4'-[(5-nitro-2,4-pyrimidinediyl)diimino]bis[2-hydroxy-, diethyl ester (9CI) (CA INDEX NAME)



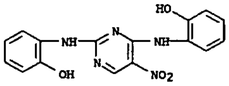
RN 116859-99-5 HCAPLUS

CN 2,4-Pyrimidinediamine, N,N'-bis(4-aminophenyl)-5-nitro- (9CI) (CA INDEX NAME)



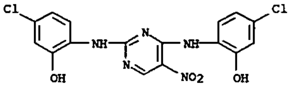
RN 116860-00-5 HCAPLUS

CN Phenol, 2,2'-[(5-nitro-2,4-pyrimidinediyl)diimino]bis- (9CI) (CA INDEX NAME)



RN 116860-01-6 HCAPLUS

CN Phenol, 2,2'-[(5-nitro-2,4-pyrimidinediyl)diimino]bis[5-chloro- (9CI) (CA INDEX NAME)

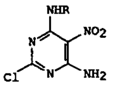


L4 ANSWER 36 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

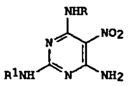
L4 ANSWER 37 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 12 May 1984

GI



I



II

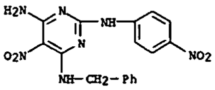
AB Reaction of 2,6-dichloro-4-amino-5-nitropyrimidine with 1-aminoadamantane gave 65% pyrimidine I (R = 1-adamantyl). Treatment of I (R = 1-adamantyl, benzyl, p-tolyl) with an amine gave 57-69% pyrimidines II (R = benzyl, p-tolyl, R1 = 1-adamantyl; R = 1-adamantyl, R1 = p-tolyl). Reaction of 2,6-dichloro-5-nitropyrimidine with 1-aminoadamantane gave 26% 2,6-bis(1-adamantylamino)-5-nitropyrimidine. II (R, R1 as above), II (R1 = p-O2NC6H4, R = PhCH2, p-O2NC6H4; R1 = p-tolyl, R = p-tolyl, 1-adamantyl), and 5-nitro-4-amino-6-benzylaminopyrimidine (III) were tested as plant growth stimulants and their activities compared with that of etalon derivs. III inhibited the growth of lettuce and oat roots and depressed the development of oat leaves. A substituted amino group at C-2 of II increased the stimulating activity of the compound

ACCESSION NUMBER: 1981:497701 HCAPLUS
DOCUMENT NUMBER: 95:97701
TITLE: Synthesis and study of the stimulating activity of adamantylamino derivatives of 2,4,6-triamino-5-nitropyrimidines and their analogs
AUTHOR(S): Tret'yakova, G. S.; Cherkasov, V. M.; Nedel'kina, N. N.; Vinogradova, T. K.
CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR
SOURCE: Fiziologicheski Aktivnye Veshchestva (1980), 12, 63-7
CODEN: FAVUAI; ISSN: 0533-1153
DOCUMENT TYPE: Journal
LANGUAGE: Russian

IT **29935-94-2 29935-96-4 29935-98-6**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(plant growth regulating activity of)

RN 29935-94-2 HCAPLUS

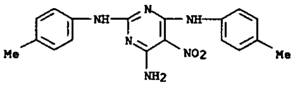
CN 2,4,6-Pyrimidinetriamine, 5-nitro-N2-(4-nitrophenyl)-N4-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 29935-96-4 HCAPLUS

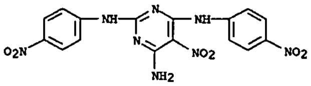
CN 2,4,6-Pyrimidinetriamine, N2,N4-bis(4-methylphenyl)-5-nitro- (9CI) (CA INDEX NAME)

L4 ANSWER 37 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 29935-98-6 HCAPLUS

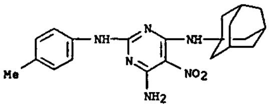
CN 2,4,6-Pyrimidinetriamine, 5-nitro-N2,N4-bis(4-nitrophenyl)- (9CI) (CA INDEX NAME)



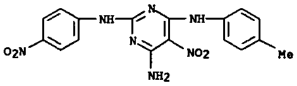
IT **77914-90-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for use of plant growth regulator)

RN 77914-90-0 HCAPLUS

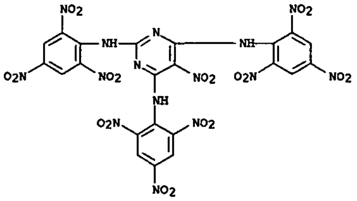
CN 2,4,6-Pyrimidinetriamine, N2-(4-methylphenyl)-5-nitro-N4-tricyclo[3.3.1.13,7]dec-1-yl- (9CI) (CA INDEX NAME)



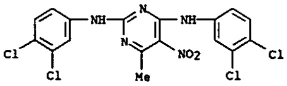
L4 ANSWER 38 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
AB When tested in 0.05-0.1% solution, 2,6-dichloro-4-amino-5-nitropyrimidine (I) [31221-68-8] showed high fungicidal and low insecticidal activities. Substitution of an amino group for the nitro group decreased the fungicidal and somewhat increased the insecticidal activities of the preparation Derivs. with amino groups substituted for chlorine at position 2 and 6 showed no fungicidal effects. 2-Chloro-4-amino-5-nitro-6-p-tolylaminopyrimidine [29955-45-1] or 2-p-nitroanilino-2,4-diamino-5-nitro-6-p-tolylaminopyrimidine [**29935-97-5**] showed great insecticidal activity.
ACCESSION NUMBER: 1973:439197 HCAPLUS
DOCUMENT NUMBER: 79:39197
TITLE: Physiological activity of some amino- and chloropyrimidines
AUTHOR(S): Tret'yakova, G. S.; Nedel'kina, N. N.; Cherkasov, V. M.
CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR
SOURCE: Fiziologicheski Aktivnye Veshchestva (1966-1992) (1972), No. 4, 93-5
CODEN: FAVUAI; ISSN: 0533-1153
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT **29935-97-5**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(insecticides)
RN 29935-97-5 HCAPLUS
CN 2,4,6-Pyrimidinetriamine, N4-(4-methylphenyl)-5-nitro-N2-(4-nitrophenyl)-(9CI) (CA INDEX NAME)



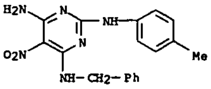
L4 ANSWER 39 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB The condensation of various aminopyrimidines (I) with picryl chloride and picryl fluoride was investigated. Most of I that can tautomerize reacted with picryl fluoride to form picryl derivs. of their imino forms (e.g. II) but picrylamino derivs. were obtained when I condensed with picryl chloride.
ACCESSION NUMBER: 1973:405309 HCAPLUS
DOCUMENT NUMBER: 79:5309
TITLE: Picrylamino-substituted heterocycles. VI. Pyrimidines
AUTHOR(S): Harris, Betty W.; Singleton, Jannie L.; Coburn, Michael D.
CORPORATE SOURCE: Los Alamos Sci. Lab., Univ. California, Los Almos, NM, USA
SOURCE: Journal of Heterocyclic Chemistry (1973), 10(2), 167-71
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **41230-78-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 41230-78-8 HCAPLUS
CN 2,4,6-Pyrimidinetriamine, 5-nitro-N,N',N''-tris(2,4,6-trinitrophenyl)-(9CI) (CA INDEX NAME)



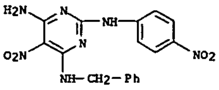
L4 ANSWER 40 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB Title compds. (I) (R = Cl, R1 = 3,4-Cl2C6H3NH, p-BrC6H4NH, p-IC6H4NH, p-O2NC6H4NH, p-AcNHC6H4O, p-BrC6H4O, p-O2NC6H4O; or R = R1 = 3,4-Cl2C6H3NH, H2NCONHNH, or H2NCSNHNH) were prepared by known methods. I had no antibacterial activity.
ACCESSION NUMBER: 1972:113158 HCAPLUS
DOCUMENT NUMBER: 76:113158
TITLE: 5-Nitro-pyrimidines
AUTHOR(S): Kartha, C. C.
CORPORATE SOURCE: Dep. Chem., Sarabhai Res. Cent., Baroda, India
SOURCE: Current Science (1972), 41(3), 101-2
CODEN: CUSCAM; ISSN: 0011-3891
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **35727-65-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35727-65-2 HCAPLUS
CN 2,4-Pyrimidinediamine, N,N'-bis(3,4-dichlorophenyl)-6-methyl-5-nitro-(9CI) (CA INDEX NAME)



L4 ANSWER 41 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB The Cl atoms in 2,4-dichloro-5-nitro-6-aminopyrimidine are not equally reactive. It is possible to replace the Cl in position 4 with RNH by reaction with RNH2 at room temperature and afterwards that at position 2 using R1NH2 either at room temperature or at 130-40° depending on the nature of R and R1. The following 2-chloro-4-substituted-amino - 6 - amino - 5 - nitropyrimidines (I) are reported (R and m.p. given): PhCH2 (A), 217-18°; (HNR =) morpholino (B), 186-7°; p-MeC6H4 (C), 239-40°; p-O2NC6H4 (D), 272-4°. II prepared at room temperature were (R, R1, and m.p. given): A, A, 183-5°; C, C, 196-8°; D, D, 316-17°. II obtained at 130-40° were: A, C, 164-5°; A, D, 248-9°; (HNR =) B, R1HN =) B, 164-5°; C, D, 216-17°; EtO2CCH2, EtO2CCH2, 148-50°.
ACCESSION NUMBER: 1971:3577 HCAPLUS
DOCUMENT NUMBER: 74:3577
TITLE: Aminolysis of 2,4-dichloro-5-nitro-6-aminopyrimidine
AUTHOR(S): Cherkasov, V. M.; Tret'yakova, G. S.; Aleksandrova, N. N.
CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR
SOURCE: Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1970), 36(7), 694-6
CODEN: UKZHAU; ISSN: 0041-6045
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT **29935-93-1P 29935-94-2P 29935-96-4P**
29935-97-5P 29935-98-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 29935-93-1 HCAPLUS
CN Pyrimidine, 4-amino-6-(benzylamino)-5-nitro-2-p-toluidino- (8CI) (CA INDEX NAME)

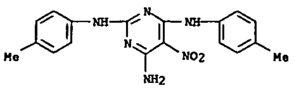


RN 29935-94-2 HCAPLUS
CN 2,4,6-Pyrimidinetriamine, 5-nitro-N2-(4-nitrophenyl)-N4-(phenylmethyl)-(9CI) (CA INDEX NAME)

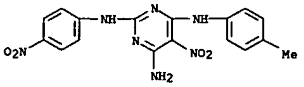


RN 29935-96-4 HCAPLUS
CN 2,4,6-Pyrimidinetriamine, N2,N4-bis(4-methylphenyl)-5-nitro- (9CI) (CA INDEX NAME)

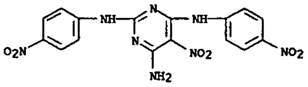
L4 ANSWER 41 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 29935-97-5 HCAPLUS
CN 2,4,6-Pyrimidinetriamine, N4-(4-methylphenyl)-5-nitro-N2-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



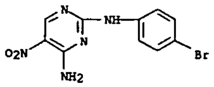
RN 29935-98-6 HCAPLUS
CN 2,4,6-Pyrimidinetriamine, 5-nitro-N2,N4-bis(4-nitrophenyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 42 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Apr 2001
AB cf. CA 63, 667g. 2,4,5-Triaminopyrimidine was found to possess confirmed antileukemic activity against L1210. This activity was not shown by structurally related compounds such as 2,4-diamino-2,4,6-triamino-, and 2,4,5,6-tetraaminopyrimidines. Preliminary investigation on the structure activity requirements for compounds in this series has been initiated. The following three classes of compounds were prepared: 2-(substituted amino)-4,5-diaminopyrimidines, 2,4-diamino-5-(substituted amino)pyrimidines, and 2,5-diamino-4-(substituted amino)pyrimidines.

ACCESSION NUMBER:	1966:27546 HCAPLUS
DOCUMENT NUMBER:	64:27546
ORIGINAL REFERENCE NO.:	64:5089e-f
TITLE:	Pyrimidines. XVI. 2,4,5-Triaminopyrimidines and related compounds
AUTHOR(S):	O'Brien, Darrell E.; Noell, C. Wayne; Robins, Roland K.; Cheng, C. C.
CORPORATE SOURCE:	Midwest Res. Inst., Kansas City, MO, USA
SOURCE:	Journal of Medicinal Chemistry (1966), 9(1), 121-6 CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE:	Journal
LANGUAGE:	English

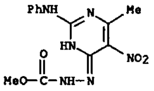
IT **5096-87-7**, Pyrimidine, 4-amino-2-(p-bromoanilino)-5-nitro-
(preparation of)
RN 5096-87-7 HCAPLUS
CN Pyrimidine, 4-amino-2-(p-bromoanilino)-5-nitro- (7CI, 8CI) (CA INDEX NAME)



L4 ANSWER 43 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB 2,4-Dichloro-5-nitropyrimidines are converted into unsym. 4-hydrazino derivs. by careful treatment with acylhydrazines. Reduction of the nitro group and cyclization affords derivs. (I) of dihydropyrimido[5,4-e]-as-triazine; one of these compds. was oxidized to the "aromatic" substance (II).

ACCESSION NUMBER:	1965:29710 HCAPLUS
DOCUMENT NUMBER:	62:29710
ORIGINAL REFERENCE NO.:	62:5280b-c
TITLE:	Polyazanaphthalenes. I. Synthesis of pyrimido[5,4-e]-as-triazines
AUTHOR(S):	Polya, J. B.; Shanks, G. F.
CORPORATE SOURCE:	Univ. Tasmania, Australia
SOURCE:	Journal of the Chemical Society (1964), (Dec.), 4986-92 CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 62:29710

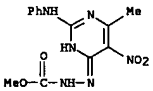
IT **1908-74-3**, Carbazic acid, 3-(2-anilino-6-methyl-5-nitro-4-pyrimidinyl)-, methyl ester
(preparation of)
RN 1908-74-3 HCAPLUS
CN Carbazic acid, 3-(2-anilino-6-methyl-5-nitro-4-pyrimidinyl)-, methyl ester (7CI, 8CI) (CA INDEX NAME)



L4 ANSWER 44 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB In the scope of investigations of the synthesis of as-triazine N-oxides, 3-amino- (I) and 3-amino-5,6-dimethyl-as-triazine (II) were oxidized with AcOOH. This led to the corresponding 5-oxo compds. and a mono-N-oxide of II whose structures, as well as those of their Ac derivs., were discussed from the standpoints of spectroscopic and dipole moment measurements. I (3 g.) in 25 ml. AcOH treated slowly with 6 ml. 30% H2O2 with ice cooling, the mixture kept 15 hrs. at room temperature, heated 1.5 hrs. at 40-5°, and cooled, the precipitate (3.2 g.) filtered and crystallized from large amts. H2O, and the appropriate fractions (identified by ir spectroscopy) combined and crystallized from H2O gave 2.0 g. 3-amino-as-triazin-5(4H)-one (III), m. above 300°. To 1.5 g. II in 13 ml. anhydrous AcOH was added 2.5 ml. 30% H2O2, the solution kept overnight, treated with 1 ml. H2O2, heated 14 hrs. at 55-60°, and cooled, and the precipitate filtered off and repeatedly crystallized from H2O to give 0.2 g. IV, m. above 300°; the mother liquor treated with a little H2O2 and concentrated to dryness in vacuo at 40-5°, this operation repeated several times, and the viscous residue dried in a desiccator and chromatographed on Al2O3 with 95% EtOH gave 0.6 g. 2-N-oxide (V) of II, m. 197.5-8.5° (Me2CO or EtOH), giving a violet FeCl3 reaction, ν (KBr) 3330, 3300, 3190, 3155, 1643, 1282 cm.-1, Rf 0.603 (1:4:5 AcOH-BuOH-H2O). V (0.1 g.) in 0.5 ml. Ac2O and 1 ml. Me2CO refluxed slowly 2 min. and then immediately concentrated in vacuo gave almost quant. 2-acetoxy-3-imino-5,6-dimethyl-as-triazine (VI), m. 141-3° (Me2CO), ν (KBr) 3180, 1710, 1210, 1195 cm.-1 CH2Cl2 (10 ml.), 2.3 g. 30% H2O2, and 2.35 g. maleic anhydride combined under ice-cooling and stirred 0.5 hr., 2.0 g. 3-acetamido-5,6-dimethyl-as-triazine (VII) in 16 ml. CH2Cl2 added dropwise, after 0.5 hr. the solution kept 3 hrs. at room temperature, filtered [from a precipitate (A)], diluted with CHCl3, washed with a little 10% aqueous Na2CO3 and then 10% aqueous NaHSO3, dried, and concentrated, and the residue chromatographed on silica gel with Me2CO gave 0.3 g. VI, m. 141-3° (Me2CO), identical (mixed m.p. and ir spectrum) with VI prepared above; crystallization of precipitate A from H2O gave 0.5 g. IV. VI (0.05 g.) in 2 ml. AcOH treated with 0.5 ml. 10% aqueous NaOH, the mixture neutralized with AcOH and concentrated in vacuo, and the residue extracted with Me2CO gave an extract containing V, identified by its ir spectrum. II (10 g.) in 40 ml. AcOH and 17 g. Ac2O heated 1 hr. at 80° and evaporated in vacuo, the residue dissolved in C6H6, and the solution washed with 10% aqueous Na2CO3 under ice-cooling and evaporated gave 7.5 g. VII, m. 131-3° (EtOAc), ν (KBr) 3260, 1730, and 1239 cm.-1 I (0.5 g.) combined with 2.5 g. Ac2O and a little AcONa and the solution heated on a water bath, treated with 2 ml. Ac2O, heated 10 min. at 130-40°, and cooled gave 3-acetamido-as-triazine-5(4H)-one (VIII), m. above 300° (H2O). VIII (1.7 g.) suspended in 30 ml. EtOH refluxed 1 hr. in an oil bath with 12 ml. 10% aqueous NaOH or 1 ml. 20% aqueous NaOH; the mixture cooled, neutralized with AcOH, and evaporated, and the residue digested with a little H2O gave (as H2O-insol.) II, identified by its ir spectrum. IV (0.4 g.) and 4 ml. Ac2O heated 5 hrs. at 130-40° and evaporated in vacuo gave quant. 3-acetamido analog (IX), m. above 300° (H2O). IX (0.2 g.) in 3 ml. EtOH containing 0.65 ml. 10% aqueous NaOH refluxed 15 min. on a water bath, cooled, and neutralized with AcOH gave 150 mg. IV, identified by its ir spectrum. HO2CCMe: NNHC(:NH)NH2 (2 g.) and 2 ml. 2N NaOH refluxed 2 hrs. in an oil bath, the mixture cooled, neutralized with AcOH, and concentrated to dryness on a water bath, and the residue crystallized from H2O gave (as a first fraction) 0.6 g. IV, identical (ir and uv spectra) with IV prepared above. The uv spectra of I, IV, V, VIII, and IX and the ir spectra of V and VI were recorded. A dipole moment of 4.31 D. was calculated for V.

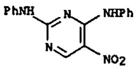
ACCESSION NUMBER:	1965:29709 HCAPLUS
DOCUMENT NUMBER:	62:29709

L4 ANSWER 44 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
ORIGINAL REFERENCE NO.: 62:5279d-h,5280a-b
TITLE: Chemistry of as-triazine. I. Structure of the oxidation products of 3-amino-as-triazines with peracetic acid
AUTHOR(S): Sasaki, Tadashi; Minamoto, Katsumaro
CORPORATE SOURCE: Coll. Sci., Tokyo
SOURCE: Chemical & Pharmaceutical Bulletin (1964), 12(11), 1329-38
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 62:29709
IT **1908-74-3**, Carbazic acid, 3-(2-anilino-6-methyl-5-nitro-4-pyrimidinyl)-, methyl ester
(preparation of)
RN 1908-74-3 HCAPLUS
CN Carbazic acid, 3-(2-anilino-6-methyl-5-nitro-4-pyrimidinyl)-, methyl ester (7CI, 8CI) (CA INDEX NAME)

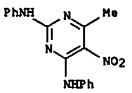


L4 ANSWER 45 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB N:CCl.N:CCl.C(NO2):CH (4.85 g.) in 20 ml. EtOH added dropwise slowly to 100 ml. aqueous MeNH2 (containing 0.15-0.2 mole MeNH2) with stirring and cooling with cold H2O, the mixture stirred 0.5 hr. at room temperature, and refrigerated for some time gave 92% N:C(NHR).N:C(NHR).C(NO2):CH (I) (R = Me), m. 251-3° (EtOH). Similarly were prepared the following I (R, % yield, and m.p. given): Et, 71, 171-2°; Pr, 95, 121-2°; iso-Pr, 92, 160-1°; Bu, 96, 129-31°; iso-Bu, 90, 137-8°; undecyl, 81, 104-5°; Ph, 99, 202-3°; benzyl, 97, 176-8°; cyclohexyl, 98, 165.5-6.5°. N:CH.N:CCl.C(NO2):CCl (4.85 g.) in 100 ml. EtOH added dropwise slowly to 6.2 g. PrNH2 in 25 ml. EtOH with stirring, refluxed 45 min., refrigerated, and diluted with H2O gave 93% N:CH.N:C(NHR).C(NO2):CNHR (II) (R = Pr), m. 62-3° (1:1 EtOH-H2O). The following II were prepared (R, % yield, and m.p. given): Me, 88, 193-4.5°; Et, 78, 83-4°; iso-Pr, 85.5, 127-8°; Bu, 57, 49-50.5°; iso-Bu, 55, 77-8°; undecyl, 67, 59-61°; Ph, 95, 168-9°; benzyl, 97, 115-16°; cyclohexyl, 90, 136-7°; CH2CH2OH, 91.5, 168-9°. 6-Me derivative of I (5.2 g.) in 50 ml. EtOH added dropwise to 10 g. PhNH2 in 200 ml. EtOH with stirring, refluxed 45 min., and cooled gave 95-100% N:C(NHR).N:C(NHR).C(NO2):CMe (III) (R = Ph), m. 144-5° (EtOH). The following III were prepared (R, % yield, and m.p. given): Me, 92, 227.5-8.5°; Et, 80, 124-5°; Pr, 85, 98-9°; iso-Pr, 95, 75-6.5°; Bu, 74, 93.5-4.0°; iso-Bu, 91, 86-8°; undecyl, 92, 75°; benzyl, 95, 118-19°; cyclohexyl, 87, 118-19.5°. I(R = Bu) (13.4 g.) in 400 ml. MeOH hydrogenated over a small amount of Raney Ni, after H absorption stopped the catalyst filtered off under N, the filtrate concentrated somewhat in vacuo at 60°, and treated with 200 ml. 5% H2SO4 gave 86% N:C(NHR).N:C(NHR).C(NH2):CH (IV) (R = Bu) sulfate, m. 208-9.5° (5% H2SO4 with C). The following IV sulfates were prepared (R, % yield, and m.p. given): Et, 44.6, 210-12°; Pr, 85.5, 210-12°; iso-Pr, 75, 207.5-9.0°; iso_Bu, 90, 210-11.5°; Ph, 84, - (free amine m. 164-6°); benzyl, 90, - (free amine m. 128-30°); cyclohexyl, 95.5, 234-5°. II (R = benzyl) (8.4 g.) in 500 ml. MeOH hydrogenated over a small amount of Raney Ni, filtered, the filtrate concentrated in vacuo, and diluted with H2O gave 84% N:CH.N:C(NHR).C(NH2):CNHR (V) (R = benzyl) m. 182-4° (40% EtOH). The following V were prepared (R, % yield, and m.p. given): Et, 58.5, 210-11°; Pr, 84, 208-9°; iso-Pr, 88, 235.5-6.5°; Bu, 92, 155.5-6.5°; iso-Bu, 93.5, 188.5-9.5°; Ph, 96, 227.5-8.0°; cyclohexyl, 88.5, 296-7°. Similarly were prepared the following N:C(NHR).N:C(NHR).C(NH2):CMe (VI) sulfates (R, % yield, and m.p. given): Me, 47, 218-20°; Et, 52, 180-2.5°; Pr, 66, 193.5-5.5°, iso-Pr, 71, 189-90°; Bu, 93, 194.5-5.5°; iso-Bu, 82, 203-5°; Ph, 97, above 300° (decomposition); benzyl, 86, 210-12°; cyclohexyl, 85, 346-7°. VI (R = Ph) sulfate (8.8 g.) suspended in 88 ml. HCONH2 (VII) gently refluxed 20-30 min., colled, dild, with 40 ml. H2O, and adjusted with aqueous NH3 to pH 7-8 (addnl. purine was obtained by concentrating the filtrate) gave 94% MeC:N.C(NHR):N.C.:C.N:CH.NR (VIII) (R = Ph), m. 263-4° (dioxane); cyclization of the free VI gave the same VIII. Similarly were prepared the following VIII (R, % yield, and m.p. given): Me, 72, 162-3.5°; Et, 84, - (HCl salt m. 230-2°); iso-Bu, 91, 125-6° benzyl, 90, 138-9.5°; cyclohexyl, 81.5, 225-7°. IV (R = Pr) sulfate (3.6 g.) in 36 ml. VII gently boiled 20-30 min. and cooled (addnl. purine was obtained by concentrating the filtrate) gave 70.2%

L4 ANSWER 45 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CH:N.C.(NHR):N.C.:C.N:CH.NR (IX) (R = Pr), m. 84-5.5° (1:5 EtOH-H2O); cyclization of the formyl derivs. of the IV gave the same IX. The following IX were prepd. (R, % yield, and m.p. given): Bu, 75, 64-5°; iso-Bu, 72, 105-5.5°; undecyl, 90, 63-4°; Ph, 85, 215-16°; benzyl, 84, 169-70°; cyclohexyl, 87, 122-4°. V (R = iso-Bu) (8 g.) in 80 ml. VII boiled gently 20 min., the VII distd. in vacuo, and the residual oil treated with dil. HCl gave 87% RHNC:N.CH:N.C:C.N:CH.NR (X) (R = iso-Bu) HCl salt, m. 219-21° (dil. HCl). The following X were prepd. (R, % yield, and m.p. given): Me, 49, 193.5-5.0°; Pr, 67, 64-5°; Bu, 85, - (HCl salt m. 184-6°); Ph, 90-5, 171-2°; benzyl, 90, 170-70.5°; cyclohexyl, 75, 68-70°. II (R = CH2CH2OH) (15 g.) in 400 ml. MeOH hydrogenated over Raney Ni, the filtered soln. evapd. in vacuo, the residual dry crude amine refluxed gently 3 hrs. with 35 ml. HC(OEt)3 and 35 ml. Ac2O, cooled, the soln. evapd. in vacuo, the residue dissolved in H2O with aq. NH3, and the soln. evapd. to dryness on a steam bath gave 52% X(R = CH2CH2OH), m. 162-3° (EtOH with C).
ACCESSION NUMBER: 1962:2399 HCAPLUS
DOCUMENT NUMBER: 56:2399
ORIGINAL REFERENCE NO.: 56:470c-i,471a-e
TITLE: Synthesis of 9-substituted purine derivatives. I. 2,9-,2,6,9-, and 6,9-substituted purines
AUTHOR(S): Goldner, H.; Carstens, E.
CORPORATE SOURCE: VEB Chem. Werke, Radebeul, Germany
SOURCE: Journal fuer Praktische Chemie (Leipzig) (1961), 12, 242-52
CODEN: JPCEAO; ISSN: 0021-8383
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 56:2399
IT **92872-53-2**, Pyrimidine, 2,4-dianilino-5-nitro- **93332-95-7**, Pyrimidine, 2,4-dianilino-6-methyl-5-nitro-
(preparation of)
RN 92872-53-2 HCAPLUS
CN Pyrimidine, 2,4-dianilino-5-nitro- (6CI, 7CI) (CA INDEX NAME)



RN 93332-95-7 HCAPLUS
CN Pyrimidine, 2,4-dianilino-6-methyl-5-nitro- (7CI) (CA INDEX NAME)



L4 ANSWER 46 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Apr 2001
AB cf. preceding abstract Cytotoxic agents were prepared by condensation of 6,2,4,5-MeCl2(O2N)C4N2 (I) with various cyclic amines. The relative activating influence of 5-NO2, 5-Cl, and 5-Br groups in 6,2,4-MeCl2C4N2R toward nucleophilic displacement of the Cl atoms was investigated. NaH (2.4 g.) and 2.15 g. aziridine (II) in 20 ml. freshly dried redistd. tetrahydrofuran bubbled through with N several min., 5.2 g. I in 50 ml. tetrahydrofuran slowly added with quant. liberation of H, the deep brown mixture hydrolyzed after 1 hr. with H2O, extracted with Et2O, and the product recrystd. from ligroine (b. 90-100°) (Norite) gave 0.9 g. bis aziridino compound, 6,5,2,4-Me(O2N)C4N2RR' (III, R = R' = aziridino) (IV), m. 120-2° (decomposition), also prepared in 1.2-g. yield by substituting anhydrous Et2O for tetrahydrofuran. KOH (3.0 g.) in 100 ml. H2O and 2.15 g. II in 50 ml. H2O stirred 30 min. with 5.2 g. I in 250 ml. ice-cold 4:1 H2O-Me2CO, the mixture stirred 16 hrs. at room temperature, the solid washed well with H2O, and dried gave 1.3 g. IV. II (4.4 g.) and 10.2 g. NEt3 in 200 ml. dry C6H6 added dropwise below 10° in 30-45 min. to 10.4 g. I in 200 ml. cold anhydrous Et2O with vigorous stirring, the thick paste diluted with 200 ml. C6H6, the mixture stirred below 10° 30 min. and 12-15 hrs. at 20°, and the filtered solution evaporated below 40° in vacuo gave 7.7 g. IV, m. 122-3° (ligroine). Concentration of the mother liquor gave addnl. 0.5 g. IV. Preliminary data on the action of IV on animal tumors was exceedingly encouraging and I was condensed with azetidine, pyrrolidine, piperidine, and morpholine to give III (R = R' = azetidino), m. 141-2° (ligroine, b. 60-80°), III (R = R' = pyrrolidino), m. 149-50° (dilute Me2CO), III (R = R' = piperidino), m. 99-100° (dilute Me2CO), and III (R = R' = morpholino), m. 162-3° (dilute Me2CO), in 63, 61, 63, and 64% yields, resp. The difference in the reactivity of the Cl atoms in I permitted the introduction of 2 different amine residues in the 2- and 4-positions. I (5.2 g.) in 200 ml. ice-cold alc. (ice-salt bath) stirred 30 min. with dropwise addition of 2.8 g. p-FC6H4NH2 in 20 ml. alc., the mixture stirred 30 min. at 20°, cooled, filtered, the filtrate concentrated, and the total product (77%) recrystd. from MeC6H11 gave 4.2 g. III (R = Cl, R' = p-FC6H4NH) (V), m. 152-4°. V (2.8 g.) and 20 ml. 40% aqueous MeNH2 heated gently on a steam bath 48 hrs. in 100 ml. absolute alc., the dry crystalline product, m. 165-75°, triturated with dilute aqueous NaOH, the product washed thoroughly with H2O, and crystallized from dilute MeOH and ligroine (b. 90-100°) gave III (R = MeNH, R' = p-FC6H4NH), m. 172-3°. V (2.82 g.) in 400 ml. Et2O stirred at 15-20° with gradual addition of 0.53 g. II and 1.1 g. NEt3 in 100 ml. absolute Et2O, the mixture stirred 18 hrs. at room temperature, filtered, the filtrate concentrated to 50 ml., heated 3 hrs. with 0.23 g. II and 0.5 g. NEt3 in 100 ml. C6H6, at 60-70°, filtered through Norit, evaporated below 35° in vacuo, the oily residue triturated with 60 ml. Et2O, and the filtrate evaporated gave 8.0 g. material, m. 116-19° (decomposition), recrystd. from petr. ether to yield anal. pure III (R = aziridino, R' = p-FC6H4NH), m. 135-7° (decomposition). I (7.8 g.) in 100 ml. MeOH treated dropwise in 15-20 min. with 14.6 g. freshly distilled furfurylamine, the mixture refluxed gently, diluted with 150 ml. C6H6, the concentrated solution (125 ml.) filtered hot, cooled, and the product (6.5 g.) recrystd. from EtOAc-ligroine gave III (R = R' = furfurylamino), m. 115-16°. I (8.6 g.) in 125 ml. warm alc. treated with 6.1 g. H2NCH2CH2OH (exothermic reaction), the mixture heated gently 48 hrs. on a steam bath, the viscous residue triturated with Me2CO, and the solid (11.5 g.) (m. 126-30°) twice recrystd. from 99:1 Me2CO-C6H6 gave 3.0 g. III (R = HO, R' = HOCH2CH2NH), m. 147.5-8.5°. Similarly, 8.62 g. I and 7.51 g. H2N(CH2)3OH in 150 ml. alc. gave a solid, which triturated with MeOH, taken up in hot dilute HCl, and basified to pH 8 with NH4OH gave 1.0 g. III [R = HO, R' = HO(CH2)3NH], m. 244.5-5.5°. Since the NO2

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group activated the Cl atoms, the effect of other 5-position substituents was studied by investigation of the 5-Cl (VI, 6,5,2,4-MeClC4N2RR') and 5-Br analogs (VII, 6,5,2,4-MeBrC4N2RR') of III. POCl3 (10 ml.), 2 ml. PhNEt2, and 1.2 g. 5-chloro-6-methyluracil refluxed 3 hrs. with stirring, the mixt. kept 24 hrs. at 20°, poured onto cracked ice, extd. with Et2O, the ext. washed with ice H2O, and the dried (MgSO4) ext. evapd. gave 1.5 g. VI (R = R' = Cl)(VIII), b0.02 55-6°. Br (4.0 g.) added dropwise in 15 min. with stirring to 3.15 g. 6-methyluracil in 100 ml. H2O, the mixt. dild. with 150 ml. H2O, refluxed 25 min., cooled to 50-60°, KOH added, the clear soln. boiled with C, the hot filtered soln. acidified with AcOH, the ppt. triturated with 200 ml. hot H2O, filtered, and the product washed with hot H2O, alc., and Et2O yielded 86% VII (R = R' = OH) (IX), m. 240-2° (decompn.). IX (41.2 g.), 300 ml. POCl3, and 80 ml. PhNEt2 heated 30 min. with stirring, refluxed 90 min., excess POCl3 removed in vacuo, the residue poured onto cracked ice, the solid washed with H2O, dried over P2O5 in vacuo, and sublimed at 40-50°/0.2 mm. 20 hrs. gave 44 g. pure VII (R = R' = Cl) (X), m. 42°, b0.3 114°. Addn. of II in Et2O to VIII in the presence of NEt3 in C6H6 yielded 78% VI (R = Cl, R' = C5H5N), m. 115-16° (Me2CO). Nucleophilic displacement of the 2-Cl and 4-Cl atoms in VIII by PhNH2, p-FC6H4NH2, and furfurylamine was readily accomplished by use of 2 equivs. amine/atom Cl to give VI (R = R' = PhNH) HCl salt, m. 284-5° (decompn.), VI (R = R' = p-FC6H4NH) HCl salt, m. 282-7° (decompn.), and VI (R = R' = furfurylamino), m. 127-8° (dil. MeOH). When only 2 equivs. p-FC6H4NH2/equiv. VIII was used, only the 4-Cl atom was replaced. VIII (1.5 g.) in 50 ml. dry Et2O and 5.5 g. p-FC6H4NH2 in 50 ml. Et2O warmed 15 min. and kept 48 hrs. at room temp. yielded 50% VI (R = Cl, R' = p-FC6H4NH) HCl salt, m. 124-5° (Et2O-petr. ether). The reactions of X paralleled those of VIII and gave the analogous compds. by displacement of both Cl atoms. X (2.42 g.) in 50 ml. Et2O stirred 4 hrs. with 1.94 g. furfurylamine and 2.02 g. NEt3 in 100 ml. Et2O, the solvent slowly evapd., the pasty mass kept 5 days at 20°, and triturated with H2O gave VII (R = R' = furfurylamino), m. 119-20° (petr. ether). Similar condensation of X with p-FC6H4NH2 and trituration with dry Et2O gave 57% residue, crystd. from MeOH and MeOH-C6H6 to give VII (R,R' = p-FC6H4NH) HCl salt, m. 243-4° (decompn.). The brown Et2O soln. evapd. and the residue crystd. from C6H6-petr. ether and Et2O-petr. ether gave 25% VII(R = Cl, R' = p-FC6H4NH), m. 143°. X (2.42 g.) in 50 ml. Et2O stirred 4 hrs. with 1.86 g. PhNH2 and 2.02 g. NEt3 in 100 ml. Et2O, the solvent slowly evapd., the pasty mass kept 24 hrs. in C6H6 at 40-60°, the insol. product taken up in MeOH, dild. with C6H6, and filtered gave the HCl salt, m. 247-9° (decompn.), crystd. from AcOH and Et2O-petr. ether to give 50% VII (R = R' = PhNH), m. 111-12°. With II only the 4-Cl atom was displaced. X (2.41 g.) in 100 ml. cold Et2O (ice bath) treated in 15 min. with 0.9 g. II and 2.1 g. NEt3 in 50 ml. Et2O, the mixt. stirred 15 hrs. at 20° with 50 ml. Et2O, the filtered soln. evapd. in vacuo, and the residue recrystd. from dil. MeOH gave VII (R = Cl, R' = aziridino), m. 127-8° (decompn.). Both Cl atoms were displaced by NaOMe. Na (5.06 g.) in 200 ml. abs. MeOH stirred 25 min. at 10-15° with 12.3 g. X in 100 ml. MeOH, the mixt. refluxed 1 hr., stirred 15 hrs. at 20°, the ppt. washed with MeOH, the mixt. refluxed 1 hr., stirred 15 hrs. at 20°, the ppt. washed with MeOH, the filtrate adjusted to pH 8 with CO2, the filtered soln. evapd., the residue triturated with H2O, and the insol. material (78%) distd. gave 7.2 g. VII (R = R' = MeO), b0.5 96-9°, m. 76-7°. The ease of displacement was dependent on the activating influence of the 5-substituent and on the nucleophilicity of the attacking reagent.

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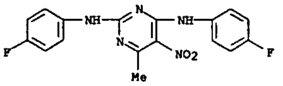
ACCESSION NUMBER: 1961:43305 HCAPLUS
DOCUMENT NUMBER: 55:43305
ORIGINAL REFERENCE NO.: 55:8422a-i,8423a-h
TITLE: Potential anticancer agents. IV. Synthesis of substituted amino- and aziridinopyrimidines
AUTHOR(S): Elderfield, Robert C.; Prasad, Raj Nandan
CORPORATE SOURCE: Univ. of Michigan, Ann Arbor
SOURCE: Journal of Organic Chemistry (1960), 25, 1583-90
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 55:43305
IT **1525-17-3**, Pyrimidine, 2,4-bis(p-fluoroanilino)-6-methyl-5-nitro-
(preparation of)
RN 1525-17-3 HCAPLUS
CN Pyrimidine, 2,4-bis(p-fluoroanilino)-6-methyl-5-nitro- (6CI, 8CI) (CA INDEX NAME)



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ED Entered STN: 22 Apr 2001
AB cf. C.A. 51, 3614g. The condensation of several 2,5-diamino-4-alkyl(and aryl)aminopyrimidines with 1,2-diketones to give 2,8-dihydro-2-imino-8-alkyl(and aryl)pteridines is described. The structures assigned to a pteridine (Ia) isolated from the eyes of Drosophila melanogaster and to luciferesceine (I), are discussed in the light of the properties of these synthetic compds. 2-Amino-4-chloro-6-hydroxypyrimidine (8.5 g.) and 25 cc. 33% alc. MeNH2 heated 4 hrs. in a sealed tube at 120°, the precipitate dissolved in 30 cc. hot dilute HCl, and the solution treated with C then with NaHCO3 gave 3.7 g. 2-amino-4-hydroxy-6-(methylamino)pyrimidine (II), plates, m. 255-7° (alc.). II (2.5 g.) in 45 cc. 2N HCl treated dropwise at 0° with 2 g. NaNO2 in 25 cc. H2O gave 2.3 g. 2-amino-4-hydroxy-6-(methylamino)-5-nitrosopyrimidine (III), red needles, m. above 300° (H2O). III (0.5 g.) in 8 cc. hot NaOH solution (containing 0.72 g. NaOH) treated 5 min. at 80° with 2 g. Na2S2O4, the mixture heated a further 20 min., and HCl added to adjust the pH to 0.5 gave 0.35 g. 2,5-diamino-4-hydroxy-6-(methylamino)pyrimidine (IV), m. 204-10° (decomposition), decomposing rapidly on attempted recrystn. IV (0.31 g.), 3 cc. AcOH, and 20 cc. H2O heated 0.5 hr. at 60-70° with 0.16 g. Ac2 gave 0.35 g. 2,8-dihydro-4-hydroxy-2-imino-6,7,8-trimethylpteridine (V), needles, decompose above 270°, pKa 5.85 (imino group) and 8.90 (OH group). V has a chromophoric system similar to that of Ia. II (0.3 g.), 3 cc. AcOH, and 20 cc. H2O heated 8 hrs. with 0.42 g. Bz2 and 12 cc. alc. gave 0.04 g. 2,8-dihydro-4-hydroxy-2-imino-8-methyl-6,7-diphenylpteridine (VI), prisms, m. above 300°. The infrared spectrum of VI was identical with that of a sample prepared from pyrazine intermediates. II (0.25 g.), 0.4 g. benzoin, 2 cc. AcOH, and 3 cc. alc. refluxed 2 hrs. gave 0.29 g. 2-amino-7,8-dihydro-4-hydroxy-8-methyl-6,7-diphenylpteridine, plates, m. above 300° (HCONMe2). 2-Amino-4-chloro-6-(methylamino)pyrimidine (VII) (6.7 g.) and 1.05 g. Na in 60 cc. alc. heated 3 hrs. at 130° in an autoclave gave 2-amino-4-ethoxy-6-(methylamino)pyrimidine (VIII), prisms, m. 123-6° (H2O). VIII (0.6 g.) in 8 cc. H2O treated at 0° dropwise with 1.1 g. diazotized p-ClC6H4NH2 in 20 cc. N HCl, then kept 5 min. at 0°, and 3.5 g. Na2CO3 added slowly gave 0.8 g. 2-amino-5-(p-chlorophenylazo)-4-ethoxy-6-(methylamino)pyrimidine (IX), orange needles, m. 169-72° (aqueous Me2CO). IX (0.6 g.) reduced in the usual way in alc. over Raney Ni and the filtrate refluxed 20 min. with 2 drops AcOH and 0.3 cc. Ac2 gave 4-ethoxy-2,8-dihydro-2-imino-6,7,8-trimethylpteridine (X), needles, m. 178-80° (aqueous alc.), not hydrolyzed by acid or alkali. VII (1.24 g.) hydrogenated in 100 cc. H2O 12 hrs. at room temperature and pressure over 0.6 g. freshly reduced 2.5% Pd-C in the presence of 0.9 g. MgO, the mixture heated to reflux, the solids removed, and 6 cc. 2N NaOH added gave 0.94 g. 2-amino-4-(methylamino)pyrimidine (XI), needles, m. 161-3.5° (iso-BuCOMe). XI (0.94 g.) in 11 cc. H2O treated at 0° with 1.4 g. p-ClC6H4NH2 diazotized with 28 cc. N HCl and 0.81 g. NaNO2, after 5 min. 3.5 g. Na2CO3 added, and the mixture left 2 hrs. at 20° gave 2.25 g. 2-amino-5-(p-chlorophenylazo)-4-(methylamino)pyrimidine (XII), red needles, m. 227-9° (alc.). XII (3 g.) in 100 cc. MeOH hydrogenated 16 hrs. at 4 atmospheric over Raney Ni and the product refluxed 0.5 hr. with 1 cc. Ac2O gave 0.5 g. crude 2,8-dihydro-2-imino-6,7,8-trimethylpteridine (XIII), needles, m. 235-40° (decomposition), pK' 5.60, evolving NH3 when heated with concentrated KOH. The ultraviolet spectrum of neutral XIII closely resembled those of the 8-alkyl-2-pteridones. There was no tendency to hydration. XIII (0.1 g.) and 3 cc. Ac2O heated 1 hr. gave 0.07 g. Ac derivative (XIV), m. 165-70° (MeOH-EtOAc). XIV absorbed at longer wavelength in the ultraviolet region than the parent XIII. This anomaly was due to the increase in conjugation provided by the Ac group; no such increase in conjugation was conferred by the Ac group in an acetamidopteridine. 2,4-Bis(methylamino)-5-nitropyrimidine (0.6 g.) in alc. reduced over Raney Ni as above and the filtered solution refluxed 10 min. with 0.5 cc. Ac2O gave 0.4 g. 2,8-dihydro-6,7,8-trimethyl-2-

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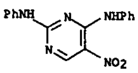
(methylimino)pteridine (XV), m. 197-8° (decompn.), pKa, 6.1, liberating MeNH2 when heated with concd. NaOH. 2,4-Dichloro-5-nitropyrimidine(0.5 g.) in 10 cc. C6H6 stirred 0.5 hr. with 4 cc. PhNH2 in 10 cc. C6H6 gave 1.3 g. crude 2,4-dianilino-5-nitropyrimidine (XVI), needles, m. 198-202° (alc.). XVI (0.3 g.) in 200 cc. alc. reduced over Raney Ni the usual way and the filtered soln. heated 20 min. with 0.3 g. Bz2, 0.3 cc. AcOH, and 3 cc. H2O gave 0.25 g. 2,8-dihydro-6,7,8-triphenyl-2-(phenylimino)pteridine, green plates, m. 225-7° (decompn.) (alc.), giving a deep green color in concd. H2SO4. XVI (0.4 g.) reduced and condensed with Ac2O gave 0.15 g. 2,8-dihydro-6,7-dimethyl-8-phenyl-2-(phenylimino)pteridine, m. 241-2° (decompn.). Comparison of the ultraviolet spectrum of I with that of XIII showed that no similarity existed. The pKa value of XIII was also much lower than that quoted for I. The structure given by Albert (C.A. 49, 2295f) is not considered to be correct. The ultraviolet absorption spectra and the pH values for many of the pteridines are given in a table.

ACCESSION NUMBER: 1958:40619 HCAPLUS
DOCUMENT NUMBER: 52:40619
ORIGINAL REFERENCE NO.: 52:7328a-i,7329a-b
TITLE: Pteridine derivatives. V. Synthesis of 2,8-dihydro-2-imino-8-alkylpteridines
AUTHOR(S): Fidler, W. E.; Wood, H. C. S.
CORPORATE SOURCE: Roy. Coll. Sci. Technol., Glasgow, UK
SOURCE: Journal of the Chemical Society (1957) 4157-62
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **92872-53-2**, Pyrimidine, 2,4-dianilino-5-nitro-
(preparation of)
RN 92872-53-2 HCAPLUS
CN Pyrimidine, 2,4-dianilino-5-nitro- (6CI, 7CI) (CA INDEX NAME)



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ED Entered STN: 22 Apr 2001

GI For diagram(s), see printed CA Issue.

AB Amino-5-arylazopyrimidines and amino-8-aryl-8-azapurines and related compds. were prepared and tested for antifolic acid activity. Compds. N:C(NH2).N:C(NH2).C(N:NR):CR' (A), N:CR.N:C(NH2).C(N:NR'):CR''(B), and C are designated by the type letter followed in parentheses by the substituents in the order R, R', and R''. 2,4-Diamino-6-chloropyrimidine (I) (1.44 g.) in 75 ml. 3N AcOH, cooled in ice H2O, and p-O2NC6H4N2Cl (from 1.38 g. p-O2NC6H4NH2) stirred 5 min., NaOAc added to pH 6-7, the mixture stirred 5 hrs., and the thick orange-red precipitate washed with H2O, dried, and recrystd. from aqueous EtOCH2CH2OH (II) gave A(p-O2NC6H4, Cl) (III), scarlet needles, m. 298-9° (decomposition). I with p-ClC6H4N2Cl formed A(p-ClC6H4, Cl) (IIIa), m. 271-2° (decomposition), fine yellow needles from aqueous II. III in dry II + Me2NH refluxed 1 hr. at 100° formed A(p-O2NC6H4, Me2N) (IV), m. 252-5°, dark maroon crystals with green luster from aqueous II. III in warm HCONMe2 and guanidine in EtOH formed a red precipitate which on fractional crystallization from aqueous II yielded IV and A(p-O2NC6H4, EtO), m. 214-15°, deep orange needles from aqueous II, forming a sparingly soluble HCl salt with dilute HCl. III refluxed with dry morpholine formed A (p-O2NC6H4, morpholino), m. 275° (decomposition), deep red prisms from aqueous II. III and dry (HOCH2CH2)2NH formed A[p-O2NC6H4, (HOCH2CH2)2N], m. 211-12° (decomposition), deep maroon plates with metallic luster from dilute EtOH, very soluble in EtOH. IIIa and guanidine with Na in II formed A(p-ClC6H4, EtOCH2CH2O), m. 161-2°, yellow lustrous silky needles from aqueous II. IIIa and Me2NH in EtOH refluxed 1 hr. or with guanidine and NaOH in EtOH refluxed 4 hrs. at 60-70° formed A(p-ClC6H4, Me2N). A(p-ClC6H4, Cl) and morpholine refluxed 1 hr. formed A(p-ClC6H4, morpholino), m. 221-2°, golden-yellow lustrous plates from aqueous II. With (HOCH2CH2)2NH was formed A [p-ClC6H4, (HOCH2CH2)2N], m. 160-1°, orange-brown prisms from dilute EtOH. The following 2,4,6-triamino-5-arylazopyrimidines were prepared by stirring a mixture of 5 g. (0.04 mole) 2,4,6-triaminopyrimidine in H2O containing 16 g. crystalline NaOAc at 0° with addition of a filtered solution of 0.04 mole of the required diazotized arylamine (aryl group, m.p., and solvent given): Ph, yellow leaflets, 262-3°, aqueous II; 2-ClC6H4, yellow needles, 290-1°, aqueous pyridine (Py); 3-ClC6H4, yellow needles, 264-5°, aqueous Py; 4-ClC6H4, yellow flat needles, 262°, aqueous II; 2-BrC6H4, golden-yellow crystals, 298-9°, aqueous II; 4-BrC6H4, yellow prisms, 261-2°, aqueous II; 2,3-Cl2C6H3, orange-yellow leaflets, 316-17°, aqueous II; 2,4-Cl2C6H3, long yellow needles, 304-5° (decomposition), aqueous Py; 2,5-Cl2C6H3, yellow needles, 319-20°, aqueous Py; 3,4-Cl2C6H3, yellow leaflets, 269-70°, aqueous Py; 2,4-Br2C6H3, orange-yellow leaflets, 328-9°, aqueous Py; 2,4,6-Br3C6H2, orange-yellow needles, 304-5° (decomposition), aqueous II; 4-MeOC6H4, orange-yellow prisms, 231-2°, aqueous II; 4-EtOC6H4, yellow needles, 280-2°, aqueous II; 4-O2NC6H4, red needles, 352-8°, AcOH; 1-C10H7, golden-brown plates, 264-5° (decomposition), aqueous II; 2-C10H7, yellow needles, 298° (decomposition), BuOH; 3-quinolyl, orange leaflets with blue luster, 315-16° (decomposition), aqueous Py. Compds. of type A (R and R' given) and type B are (R, R', and R'' given): A (p-ClC6H4, HO), yellow microcryst. powder, m. 314-15°; A (p-BrC6H4, HO), yellow crystals from aqueous Py and aqueous II; B (HO, p-ClC6H4, HO), fine yellow powder; A(p-ClC6H4, H), yellow needles from aqueous II, m. 282-3° (decomposition) (reported 271-2°); B (H, p-ClC6H4, HO), orange needles, m. 300° (from aqueous II). 4,6-Diamino-5-(p-chlorophenylazo)-2-thiopyrimidine, yellow needles, m. 278-9°(decomposition) (from aqueous Py), and 4,6-diamino-5-(p-chlorophenylazo)-2-

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(p-chlorophenylthio)pyrimidine, yellow feathery needles, m. 211-12° (from aq. EtOH). B(H, p-ClC6H4, H2N), flat yellow needles, m. 299-300° (decompn.) (from aq. II). The following C were prepd. in quant. yield from the corresponding N:CR''.N:CR'.C(N2R):CNH2 in pyridine and H2O contg. CuSO4 refluxed with a stream of O until the color changed from greenish yellow to blue, and the hot soln. allowed to stand to complete pptn. [R, m.p., and solvent (a = 20% aq. HCO2H, b = 80% aq. HCO2H, c = HCONH2) given; R' and R'' = H2N unless otherwise stated]: Ph, 344-5° (decompn.), a; o-ClC6H4, 283-4°, a; m-ClC6H4, 350° (decompn.), a; p-ClC6H4, above 360°, a; o-BrC6H4, 271-2°, 10% a; p-BrC6H4, C10H8N7Br. 0.5HCO2H, above 360°, a; 2,3-Cl2C6H3, C10H7N7Cl2.0.5H2O, 287-8°, a; 2,4-Cl2C6H3, 320-1°, a; 2,5-Cl2C6H3, 312-13°, a; 3,4-Cl2C6H3, above 360°, a; 2,4-Br2C6H3, C10H7N7Br2.HCO2H, 279-81° (decompn.), a; 2,4,6-Br3C6H2, 286-7°, H2O-EtOH; p-EtOC6H4, C12H13N7O.0.25HCO2H, 310-11°, a; 1-C10H7, 290-1°, a; p-ClC6H4 (R' = HO), above 360°, b; p-BrC6H4 (R' = HO), above 360°, b; p-ClC6H4 (R' = Me2N), HCl salt, 287-8°, 2N HCl; p-O2NC6H4 (R' = Me2N), 316-18°, c; p-ClC6H4 (R'' = p-ClC6H4S), 325-6° (decompn.), b; p-ClC6H4 (R'' = H), 367° (decompn.), AcOH; p-ClC6H4 (R' = HO, R'' = H), 339-40°, aq. II. The HO derivs. refluxed with P2S5 in dry pyridine formed 8-(p-chlorophenyl)-6-thio-8-azapurine, pale golden lustrous needles, m. 357-8° (decompn.) (from aq. Py and C); and 2-amino (from Py and C). A (3-quinolyl, H2N) refluxed with H2O, Py, and CuSO4.5H2O in H2O with an O stream until clear blue formed C (3-quinolyl, HO, H2N), pale cream solid, m. above 360° (repptd. from 2N HCl with 2N NH3). Closure of the ring in the triamino deriv. formed C (3-quinolyl), pale cream solid, m. above 360° (from propylene glycol + C). 2,6-Diamino-3-(4-chlorophenylazo)pyridine, Py, CuSO4.5H2O in H2O, and O formed 5-amino-2-(4-chlorophenyl)triazolo[4',5'-2,3]pyridine, long felted needles from aq. II changing to pale yellow prismatic needles, both forms m. 258-9°. 2-Amino-4-anilino-5-nitropyrimidine, yellow needles, m. 206-7° (from 4-anilino-2-chloro-5-nitropyrimidine), + SnCl2 formed 2,5-diamino-4-anilinopyrimidine, di-HCl salt, m. 249-50° (decompn.); monopicrate, m. 249-50° (decompn.). Diazotization of the HCl salt yielded 2-amino-9-phenyl-8-azapurine, rosettes of needles, m. 167-8° (from H2O-MeOH and C). 2-Amino-4-anilino-6-methyl-5-nitropyrimidine, yellow needles, m. 192-3° (from BuOH) (from the 2-Cl compd.), was reduced with SnCl2 to the 2,5-diamino compd. [di-HCl salt, lustrous needles, m. 239-40°; monopicrate, orange-yellow leaflets m. 252-3° (decompn.)], diazotized to 2-amino-6-methyl-9-phenyl-8-azapurine, needles, m. 188-9° (from aq. MeOH). 2,4-Dichloro-5-nitropyrimidine in EtOH at -10° and ClC6H4NH2 in EtOH formed 2-chloro-4-(4-chloroanilino)-5-nitropyrimidine, yellow needles m. 150-1° (from EtOH), which reacted with satd. NH3 in EtOH in a sealed tube at 100° for 3 hrs. to form 2-amino-4-(4-chloroanilino)-5-nitropyrimidine, golden-yellow leaflets m. 241° (from BuOH), which was reduced with SnCl2 to 2,5-diamino-4-(4-chloroanilino)pyrimidine, [di-HCl salt (1H2O), m. 286-7° (decompn.); monopicrate, lemon-yellow rosettes m. 256° (decompn.)]. 2-Amino-9-(4-chlorophenyl)-8-azapurine, rosettes of fine white needles, m. 236° (from aq. MeOH). 8-Azapurine, m. 175°, from 4,5-diaminopyrimidine refluxed with AmNO2. 2,6-Diaminopyridine, in 2N HCl cooled in ice, stirred and treated slowly with p-ClC6H4N2Cl formed 2,6-diamino-3-(4-chlorophenylazo)pyridine, yellow prisms, m. 184-5° (from aq. EtOH). Removal of the aryl or aryl and amino groups from diamino-8-aryl-8-azapurines gave inactive compds. The position of the aryl group in the aryl-8-azapurine relative to the

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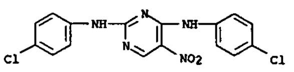
pyrimidine ring is important. Substitution of a pyrimidine by a pyridine ring led to inactivity. Screened with Streptococcus faecalis and pteroylglutamic acid 23 arylazopyrimidines and 15 8-azapurines showed antifolic acid activity, C (R' = R'' = NH2, R = 2,4-BrC6H3) showing about 1/50 the potency of A-methopterin.

ACCESSION NUMBER:	1957:56795 HCAPLUS
DOCUMENT NUMBER:	51:56795
ORIGINAL REFERENCE NO.:	51:10531i,10532a-i,10533a-h
TITLE:	Structure-activity relations in two new series of antifolic acids
AUTHOR(S):	Timmis, G. M.; Felton, D. G. I.; Collier, H. O. J.; Huskinson, Patricia L.
SOURCE:	Journal of Pharmacy and Pharmacology (1957), 9, 46-67 CODEN: JPPMAB; ISSN: 0022-3573
DOCUMENT TYPE:	Journal
LANGUAGE:	Unavailable
OTHER SOURCE(S):	CASREACT 51:56795

IT **101727-04-2**, Pyrimidine, 2,4-bis(p-chloroanilino)-5-nitro-
(preparation of)

RN 101727-04-2 HCAPLUS

CN Pyrimidine, 2,4-bis(p-chloroanilino)-5-nitro- (6CI) (CA INDEX NAME)



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ED Entered STN: 22 Apr 2001

GI For diagram(s), see printed CA Issue.

AB Reaction of some chloro-5-nitropyrimidines with C5H5N (I), 2-aminopyridine (II), and 2-amino-3-methyl- (III) or 2-amino-4-methylpyridine (IV) gave in general, quaternary salts formed via the 2-Cl substituent of the pyrimidine; the 4-Cl substituent (when present) condensed normally with the NH2 group. When 2-amino-6-methylpyridine (V) reacted with 2,4-dichloro-6-methyl- (VI) or 2,4-dichloro-5-nitropyrimidine (VII) no quaternary salt was formed; condensation occurred between the NH2 group and successively, the 4- and the 2-Cl substituent. The replacement of aminopyridyl substituent in 2-position of the pyrimidine quaternary salts by alkoxy and NH2 groups was studied. VII (4.2 g.) in MeOH treated with ice-cold solution of 4.1 g. II in MeOH, after 2 hrs. at 0° the solids collected, and washed gave 0.9 g. 2-chloro-5-nitro-4-(2-pyridylamino)pyrimidine (VIII) as prisms, m. 156° (from EtOH), and 3.6 g. 2-amino-1-[5-nitro-4-(2-pyridyl-amino)-2-pyrimidyl]pyridinium chloride (IX) as yellow needles, m. 249° (decomposition) (from H2O or dilute HCl). IX afforded the bromide, m. 262° (decomposition) (from H2O), and the iodide as orange needles, m. 252° (decomposition) (from H2O). IX separated quant. when 3 moles II were used. VIII (0.2 g.) and 0.4 g. II in hot MeOH gave IX immediately. VII and II in hot MeOH gave IX but continued refluxing gave a clear solution which yielded 2-methoxy-5-nitro-4-(2-pyridylamino)pyrimidine (X), m. 148°. VIII refluxed 2 hrs. with Na in MeOH gave X. Similarly VIII yielded the 2-ethoxy analog (XI), m. 131°. XI was also obtained when IX was refluxed with II in EtOH. VI treated with II in ice-cold MeOH gave exclusively the quaternary chloride (XII) as yellow needles, m. 215° (decomposition). VI (1 mole) and 4 moles II refluxed in MeOH gave 2-methoxy-6-methyl-5-nitro-4-(2-pyridylamino)pyrimidine (XIII) as prisms, m. 137°. Reaction in EtOH gave the ethoxy analog of XIII, m. 113-14° (from EtOH). 2-Chloro-4-amino-5-nitropyrimidine (XIV) (0.5 g.) and 1 g. II heated 1 hr. at 120-30°, the melt treated with 50% EtOH, and the solid dissolved in N/20 HCl, and precipitated with NH3 gave 4-amino-5-nitro-2-(2-pyridylamino)pyrimidine as needles, m. 276° (from aqueous C5H5N). VIII refluxed 2 hrs. with MeOH-NH3 gave 2-amino-5-nitro-4-(2-pyridylamino)pyrimidine (XV), plates, m. 251-2° (from BuOH). IX (0.5 g.) refluxed 2 hrs. with concentrated NH3 in MeOH gave 0.3 g. XV. IX (0.5 g.) refluxed 2 hrs. in EtOH containing 2 ml. PhNH2 yielded 2-anilino analog (XVI) of XV, m. 218° (from EtOH). A better solvent for this reaction was 50% aqueous Me2CO. XVI was also formed by shaking IX with EtOH and PhNH2 2 hrs. at room temperature, or by heating IX with PhNH2 for 10 min. at 125°. XII (1 g.) heated 1 hr. in a sealed tube at 100° with saturated MeOH-NH3 gave 2-amino-6-methyl-5-nitro-4-(2-pyridylamino)pyrimidine (XVII) as prisms, m. 230° (from BuOH). 2-Amino-4-chloro-6-methyl-5-nitropyrimidine and II heated 0.5 hr. at 125° gave XVII. V (1.9 g.) left 2 hrs. at 0° with 2 g. VII gave 2 g. 2-chloro-4-(6-methyl-2-pyridylamino)-5-nitropyrimidine (XVIII), m. 144° (from EtOH). V (4 moles) refluxed 5 hrs. with VII in MeOH gave 2,4-di(6-methyl-2-pyridylamino)-5-nitropyrimidine, m. 318° (from AcOH). III and VII in MeOH at 0° with 2-3 moles of the pyridine gave the salt as prisms, m. 250° (decomposition) (from H2O). If 1 mole of VII was refluxed with 4 moles III in MeOH the product was 2-methoxy-4-(3-methyl-2-pyridyl-amino)-5-nitropyrimidine, m. 110° (from H2O or light petroleum). VII treated with 3 moles IV in cold MeOH gave the quaternary salt as prisms, m. 237-8° (from H2O). When VII was refluxed with 4 moles IV in hot MeOH 2-methoxy-4-(4-methyl-2-pyridylamino)-5-nitropyrimidine was formed, m. 180° (from BuOH). VI (2.08 g.) left 1 hr. at 0° with 2.16 g. V in MeOH and Et2O gave 2 g. 2-chloro-6-methyl-4-(6-methyl-2-pyridylamino)-5-nitropyrimidine (XIX), m. 120° (from EtOH). VI refluxed with 4 moles V in MeOH gave 6-methyl-2,4-di(6-methyl-2-pyridylamino)-5-nitropyrimidine as yellow needles, m. 180° (from EtOH). 6-Amino-2,4-dichloro-5-

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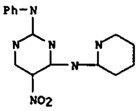
nitropyrimidine (1 g.) and 1.4 g. II kept 4 days at room temp. in Me2CO, evapd. and extd. with hot H2O gave a residue A (0.3 g.). The hot filtrate was treated with C, filtered, and cooled to give 1 g. solid B. Solid A yielded 6-amino-2-chloro-4-(2-pyridylamino)-5-nitro-pyrimidine (XX) as yellow needles, m. 239° (from BuOH). Solid B yielded the quaternary chloride as prisms, m. 271° (decompn.) (from EtOH-Et2O), and the iodide as orange prisms, m. 265° (decompn.) (from H2O). Reaction with 2 moles of II in ice-cold EtOH gave only XX. VIII (0.5 g.) reacted with 0.7 ml. I in C6H6 giving 1-[5-nitro-4-(2-pyridylamino)-2-pyrimidyl]pyridinium chloride as prisms, m. 220° (decompn.). 4-Anilino-2-chloro-5-nitropyrimidine (0.3 g.) and 0.5 g. I in C6H6, and the salt treated with NaI in H2O yielded the pyridinium iodide, plates, m. 215° (decompn.). 2-Chloro-4-(6-methyl-2-pyridylamino)-5-nitropyrimidine and I gave the chloride, m. 200° (decompn.) (from EtOH-Et2O). XIX and I similarly treated and the salt then treated with NaI gave the quaternary iodide as scarlet needles, m. 224° (decompn.) (from H2O). 1-(5-Nitro-4-amino-2-pyrimidyl)pyridinium chloride (XXI, R2 = NH2, R1 = R3 = H) was prepd. from the components in Me2CO as buff needles, m. 255-6° (decompn.). Similarly were prepd. the following analogs of XXI: R2 = R3 = NH2, R1 = H, rods, m. 273-4° (decompn.); R2 = PhNH, R1 = H, R3 = NH2, prisms, m. 200-2° (decompn.) (from EtOH-Et2O) [the iodide, orange rods, m. 213-14° (decompn.)]; R2 = 6-methyl-2-pyridylamino, R1 = H, R3 = NH2, yellow prisms, m. 222-3° (decompn.) [the iodide, m. 252° (decompn.)].

ACCESSION NUMBER: 1956:56933 HCAPLUS
DOCUMENT NUMBER: 50:56933
ORIGINAL REFERENCE NO.: 50:10729d-i,10730a-h
TITLE: Quaternary salts from 2-chloro-5-nitropyrimidines. I. Preparation and some reactions
AUTHOR(S): Spickett, R. G. W.; Timmis, G. M.
CORPORATE SOURCE: Roy. Cancer Hosp., London
SOURCE: Journal of the Chemical Society (1955) 4354-9
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **874494-38-9**, Pyrimidine, 2-anilino-5-nitro-4-(2-pyridylamino)-
(preparation of)
RN 874494-38-9 HCAPLUS
CN Pyrimidine, 2-anilino-5-nitro-4-(2-pyridylamino)- (5CI) (CA INDEX NAME)

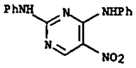


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L4 ANSWER 50 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Apr 2001
AB cf. C.A. 49, 12130h, 13256a. Adding 10 g. PhNH2 in 200 cc. absolute EtOH to 5 g. 2,4-di-chloro-5-nitropyrimidine (I) in 20 cc. absolute EtOH with stirring and refluxing the mixture 45 min. give 94% 2,4-di-anilino-5-nitropyrimidine (II), fluffy light yellow needles, m. 203-4°. Reducing 2 g. II in 150 cc. absolute EtOH 3-6 h. with 2 g. Raney Ni gives 70% 2,4-dianilino-5-aminopyrimidine (III), m. 165-8° (decomposition). Adding 0.16 g. NaNO2 to 0.57 g. III dissolved in 400 cc. 5% AcOH at 10-20°, stirring the mixture 15 min., and adjusting the solution to pH 8-9 give 62% 3-phenyl-5-anilino-1H-v-triazolo[d]pyrimidine, light green needles, m. 195°. Refluxing 0.91 g. III in 10 cc. 90% HCO2H 15 min., evaporating the HCO2H, dissolving the residue in 5 cc. H2O, and adjusting the solution to pH 7-8 with NH4OH give 0.97 g. 2,4-dianilino-5-formamidopyrimidine (IV), needles, m. 193.5-5° (the rate of heating affects the m.p.; another determination gives 187-9°, resolidifying and remelting at 215°). Gently refluxing 1 g. IV 15 min. with 10 cc. HCO-NH2, adding 10 cc. H2O, and adjusting the solution to pH 7-8 give 92% 2-anilino-9-phenylpurine, needles, m. 215-16°. Adding slowly 5 g. I in 20 cc. EtOH to 8.5 cc. PrNH2 in 100 cc. EtOH and refluxing the mixture 0.5 h. give 91% 2,4-di-propylamino-5-nitropyrimidine (V), m. 121-2°, which (2 g.) is reduced in 115 cc. MeOH with 2 g. Raney Ni 2-3 h. at 30 lb. and the residue of the filtered and evaporated solution treated with H2SO4, giving 72% 2,4-dipropylamino-5-aminopyrimidine sulfate (VI). Stirring 1.84 g. VI in 200 cc. H2O containing 2 drops H2SO4 0.5 h. at 10-20° with 0.55 g. NaNO2 and adjusting the solution to pH 7-8 give 49% 3-propyl-5-propylamino-1H-v-triazolo[d]pyrimidine, long needles, m. 97.5-8°. Refluxing the reduction product of 2.65 g. V with 15 cc. HCO2H, adding 5 cc. H2O, and adjusting the solution to pH 7-8 give 1.5 g. 2,4-dipropylamino-5-formamidopyrimidine, shiny platelets, m. 159.5-60.5°, which (0.94 g.), refluxed 15 min. with 10 cc. HCONH2, gives 0.35 g. 2-propylamino-9-propyl-purine, m. 84-5°. Refluxing 8.25 g. 2-chloro-4-(2-hydroxyethylamino)-5-nitropyrimidine in 120 cc. EtOH saturated with NH3 in an NH3 atmospheric gives 93% 2-amino-4-(2-hydroxyethylamino)-5-nitropyrimidine (VII), m. 192-4°. Reduction of 2 g. VII in MeOH 1-2 h. with Raney Ni at 30 lb. and acidification of the filtered and concentrated solution with H2SO4 give 1.46 g. sulfate, m. 169-70°, which, treated with NaNO2, gives 65% 3-(2-hydroxyethyl)-5-amino-1H-v-triazolo[d]pyrimidine, m. 220-1°. Reducing 4 g. VII with 5 g. Raney Ni in 200 cc. MeOH and concentrating the filtered solution give 1 g. 2,5-diamino-4-(2-hydroxyethylamino)pyrimidine, m. 140-1.5°, which, refluxed 15 min. with 10 cc. HCO2H, gives 0.3 g. 5-formamido derivative (VIII), m. 165-6°. Refluxing 0.55 g. VIII 15 min. with 10 cc. HCONH2 gives 0.3 g. 2-amino-9-(2-formyloxyethyl)purine, needles, m. 172-3°. Adding AcOH dropwise to 2 g. 2-mercapto-4,5-diaminopyrimidine in 1.2 l. H2O containing 2 g. NaNO2 at 30° gives 1.6 g. 5-mercapto-1H-v-triazolo[d]pyrimidine, exploding on a m.p. block.

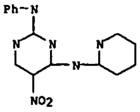
ACCESSION NUMBER: 1956:20104 HCAPLUS
DOCUMENT NUMBER: 50:20104
ORIGINAL REFERENCE NO.: 50:4159i,4160a-f
TITLE: Purines. V. The preparation of certain 2,9-substituted purines and azapurines
AUTHOR(S): Dille, K. L.; Sutherland, M. L.; Christensen, B. E.
CORPORATE SOURCE: Oregon State Coll., Corvallis
SOURCE: Journal of Organic Chemistry (1955), 20, 171-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

L4 ANSWER 50 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
IT **92872-53-2**, Pyrimidine, 2,4-dianilino-5-nitro-
(preparation of)
RN 92872-53-2 HCAPLUS
CN Pyrimidine, 2,4-dianilino-5-nitro- (6CI, 7CI) (CA INDEX NAME)



L4 ANSWER 51 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Apr 2001
AB cf. Turitsyna and Vompe, C.A. 45, 3846h. 2,4-Dichloro-5-nitropyrimidine (I) and cold NH3 give the 4-amino (II) and under more vigorous conditions the 2,4-diamino compound (III); I and esters of α-amino acids or α-amino ketones give the corresponding 4- with some 2,4-disubstituted pyrimidines. 2,4-Dichloro-6-methyl-5-nitropyrimidine (IV) reacts similarly. I and 2-C5H4NNH2 (V) in ice-cold MeOH give some 2-chloro-5-nitro-4-(2-pyridylamino)pyrimidine (VI), m. 148° and as main product the water-soluble 2-amino-1-[5-nitro-4-(2-pyridylamino)-2-pyrimidyl]pyridinium chloride (VII), m. 234-6° (decomposition). VII is also obtained from VI with V (or from I and 3 mols. V) in boiling MeOH. IV and V give only the 6-methylpyrimidyl homolog (VIII) of VII. The 2-Cl is involved in the salt formation: 2-amino-4-chloro-6-methyl-5-nitropyrimidine with V gives only 2-amino-6-methyl-5-nitro-4-(2-pyridylamino)pyrimidine (IX) (also obtained from VIII and MeOH-NH3 at 100°); 4-anilino-2-chloro-5-nitropyrimidine (from I and PhNH2 in cold MeOH) and V give 4-anilino-5-nitro-2-(2-pyridylamino)pyrimidine, which is different from the 2-anilino-4-(2-pyridylamino) isomer, m. 207-8°, obtained from VII and PhNH2. VII or VIII boiled in MeOH with excess V, base, Et3N, or NaOMe give 2-methoxy-5-nitro-4-(2-pyridylamino)pyrimidine and its 6-Me homolog (X), resp.; similarly, in EtOH they give the 2-EtO analogs. VII with boiling MeOH and NH3 gives 2-amino-5-nitro-4-(2-pyridylamino)pyrimidine (XI), m. 240-2°; with 10% Et2NH in EtOH gives the 2-diethylamino derivative of XI, m. 133-4°; with 10% C5H10NH in EtOH gives the 2-(1-piperidyl) derivative of XI, m. 164°. VIII and boiling MeOH-NH3 give X (reaction in a sealed tube gives IX). Analogous reactions take place when 3-amino and 4-aminopyridines are used for V. 2-Amino-6-methylpyridine and I give 2-chloro-5-nitro-4-(6-methyl-2-pyridylamino)pyrimidine (XII) and on more vigorous treatment the 2,4-bis(6-methyl-2-pyridylamino) derivative XII does not form salts with quinoline or 2-methylpyridine (possibly because of steric conditions). VII and alkali give a yellow product (IX), m. 135-40° (decomposition), which reverts to VII with dilute HCl; IX may be an anhydro base of VII, 5-nitro-2-(1,2-dihydro-2-imino-1-pyridyl)-4-(2-pyridylamino)pyrimidine.

ACCESSION NUMBER: 1952:48660 HCAPLUS
DOCUMENT NUMBER: 46:48660
ORIGINAL REFERENCE NO.: 46:8121g-i,8122a-c
TITLE: Quaternary salts from 2-chloro-5-nitropyrimidines, and their reactions
AUTHOR(S): Spickett, R. G. W.; Timmis, G. M.
CORPORATE SOURCE: Roy. Cancer Hosp., London
SOURCE: Chemistry & Industry (London, United Kingdom) (1951) 937-9
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **874494-38-9**, Pyrimidine, 2-anilino-5-nitro-4-(2-pyridylamino)-
(preparation of)
RN 874494-38-9 HCAPLUS
CN Pyrimidine, 2-anilino-5-nitro-4-(2-pyridylamino)- (5CI) (CA INDEX NAME)



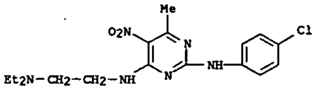
L4 ANSWER 51 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

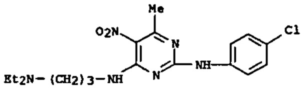
L4 ANSWER 52 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Apr 2001
AB See Brit. 587,550 (C.A. 42, 2627c). Not included in this abstract is 4-p-chloroanilino - 2 - (3 - dibutylaminopropylamino) - 6-methylpyrimidine(di-HCl salt, m. 171-3°).
ACCESSION NUMBER: 1948:34449 HCAPLUS
DOCUMENT NUMBER: 42:34449
ORIGINAL REFERENCE NO.: 42:7346e-f
TITLE: Pyrimidine derivatives
INVENTOR(S): Curd, Francis H. Swinden; Hall, Margaret I.; Owen, Edmund C.; Rose, Francis L.; Tuey, George A. P.
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2443305		19480615	US	

IT **873375-60-1**, Pyrimidine, 2-p-chloroanilino-4-(2-diethylaminoethylamino)-6-methyl-5-nitro- **873375-82-7**, Pyrimidine, 2-p-chloroanilino-4-(3-diethylaminopropylamino)-6-methyl-5-nitro-
(preparation of)
RN 873375-60-1 HCAPLUS
CN Pyrimidine, 2-p-chloroanilino-4-(2-diethylaminoethylamino)-6-methyl-5-nitro- (5CI) (CA INDEX NAME)



RN 873375-82-7 HCAPLUS
CN Pyrimidine, 2-p-chloroanilino-4-(3-diethylaminopropylamino)-6-methyl-5-nitro- (5CI) (CA INDEX NAME)

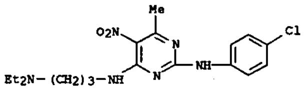


L4 ANSWER 53 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Apr 2001
AB The compds. are prepared by heating equimol. proportions of an arylamine, the quinazoline, and a mineral acid (a flight excess of acid can be used) in aqueous medium. 2-Chloro-4-(3-diethylaminopropylamino)quinazoline-2H2O and p-anisidine (130-40° for 3 hrs.) yield 2-p-methoxyanilino-4-(3-diethylaminopropylamino)quinazoline, colorless needles m. 114-15°. Similar reactions yield the 2-anilino, prisms, m. 112-14°, 2-p-toluidino, needles, m. 94°, 2-(2-naphthylamino), needles m. 141°, and 2-p-chloroanilino analog, prisms, m. 127°. 2-Chloro-4-(2-diethylamioethylamino)quinazoline-H2O (I) and p-MeSC6H4NH2 (130-40° for 3 hrs.) yield the 2-[(p-methylmercapto)anilino] analog (HCl salt m. 130-1°); 2-C10H7NH2 yields the 2-(2-naphthylamino) analog, needles, m. 126°. p-ClC6H4NH2, and AcOH, refluxed 2 hrs., yield the 2-p-chloroanilino analog, small white prisms m. 111-12° (HCl salt m. 254-5°). In the same way are obtained the following 2-(p-chloroanilino)-4-(R-amino)quinazolines from the corresponding 2-Cl compds.: R = (2-dimethylaminoethyl) (2HCl m. 267-8°); (3-dimethylaminopropyl) (2HCl m. 256-8°); (4-diethylaminobutyl) (2HCl m. 260-2°); (3-butylaminopropyl) (2HCl m. 254-6°); [3-(1-piperidyl)propyl] (2HCl m. 285-6°). I, 6,2-BrC10H6NH2, and AcOH, refluxed 2 hrs., yield the 2-(6-bromo-2-naphthylamino) analog (2HCl m. 284-5°); 4,8,2-Cl2C10H5NH2 yields the 2-(4,8-dichloro-2-naphthylamino) analog (2HCl m. 284°). 2,7-Dichloro-4-(2-diethylaminoethylamino)quinazoline, p-ClC6H4NH2, and AcOH, refluxed 2 hrs., yield the 7-chloro-2-p-chloroanilino analog, m. 121-2° (2HCl m. 280-3°). The appropriate aminoquinazolines yield the following 2-p-chloroanilino-4-(2-diethylaminoethylamino)quinazolines: 6-Cl (2HCl m. 282°); 7-Me (2HCl m. 264°); 7-MeO (2HCl m. 230-2°); 6-MeO (2HCl m. 248-9°); 8-MeO (2HCl m. 274-5°); 7-NO2 m. 160°; 6,7-benzo (2HCl m. 286-7°); 6,7-di-MeO, m. 255-6°. 2-p-Chloroanilino-4-[3-(1-piperidyl)propylamino]quinazoline (2HCl m. 285-6°); 4-(2-dimethylaminoethylamino) analog (2HCl m. 267-8°); 2-p-chloroanilino-4-(2-diethylaminoethylamino)-5-methoxyquinazoline(2HCl m. 187-8°); 2-p-nitroanilino 4-(2-diethylaminoethylamino)quinazoline(2HCl m. 286-7°); 2-p-chloroanilino-6-nitro-4-(2-diethylaminoethylamino)quinazoline m. 200-1° (2HCl m. 266°); the 6-amino analog(3HCl-5H2O m. 180°); 2-p-chloroanilino-4-[methyl(2-diethylaminoethyl)amino]quinazoline(2H2O, colorless crystals m. 76°); 2-N-ethylanilino-4-(2-diethylaminoethylamino)quinazoline m. 110°.
ACCESSION NUMBER: 1948:21486 HCAPLUS
DOCUMENT NUMBER: 42:21486
ORIGINAL REFERENCE NO.: 42:4615e-i,4616a-b
TITLE: Quinazoline derivatives
INVENTOR(S): Curd, Francis H. S.; Landquist, Justus K.; Raison, Clifford G.; Rose, Francis L.
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 587936		19470509	GB	

IT **873375-82-7**, Pyrimidine, 2-p-chloroanilino-4-(3-diethylaminopropylamino)-6-methyl-5-nitro-
(preparation of)
RN 873375-82-7 HCAPLUS
CN Pyrimidine, 2-p-chloroanilino-4-(3-diethylaminopropylamino)-6-methyl-5-nitro- (5CI) (CA INDEX NAME)

L4 ANSWER 53 OF 57 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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L4   ANSWER 54 OF 57  HCAPLUS  COPYRIGHT 2006 ACS on STN
ED   Entered STN:  22 Apr 2001
AB   See Brit. 592,928 (C.A. 42, 2291a).  In addition to the compds. listed in the
     abstract, the following were not previously described: 2-(6-bromo-2-
     naphthylamino)-4-[3-(1-piperidyl)propylamino]-6-methylpyrimidine (di-HCl
     salt, m. 256-8° ); 2-(2-naphthylamino)-4-(4-diethylamino-1-
     methylbutylamino)-6-methylpyrimidine (di-HCl salt m. 268-70°
     (decomposition)); 2-(p-chloroanilino)-4-(2-diethylaminoethylamino)-6-methyl-5-
     nitropyrimidine, m. 146-8°; and the 4-(3-diethylaminopropylamino)
     analog, m. 94-6°.
ACCESSION NUMBER:        1948:21485  HCAPLUS
DOCUMENT NUMBER:         42:21485
ORIGINAL REFERENCE NO.:  42:4615c-e
TITLE:                   Pyrimidines
INVENTOR(S):             Curd, Francis H. S.; Raison, Clifford G.; Rose,
                         Francis L.
PATENT ASSIGNEE(S):      Imperial Chemical Industries Ltd.
DOCUMENT TYPE:           Patent
LANGUAGE:                Unavailable
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE       APPLICATION NO.        DATE
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     US 2437683                 19480316   US
IT   873375-60-1, Pyrimidine, 2-p-chloroanilino-4-(2-
     diethylaminoethylamino)-6-methyl-5-nitro- 873375-82-7,
     Pyrimidine, 2-p-chloroanilino-4-(3-diethylaminopropylamino)-6-methyl-5-
     nitro-
        (preparation of)
RN   873375-60-1  HCAPLUS
CN   Pyrimidine, 2-p-chloroanilino-4-(2-diethylaminoethylamino)-6-methyl-5-
     nitro- (5CI)  (CA INDEX NAME)
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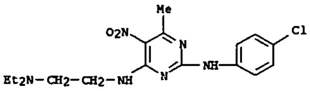

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RN   873375-82-7  HCAPLUS
CN   Pyrimidine, 2-p-chloroanilino-4-(3-diethylaminopropylamino)-6-methyl-5-
     nitro- (5CI)  (CA INDEX NAME)
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